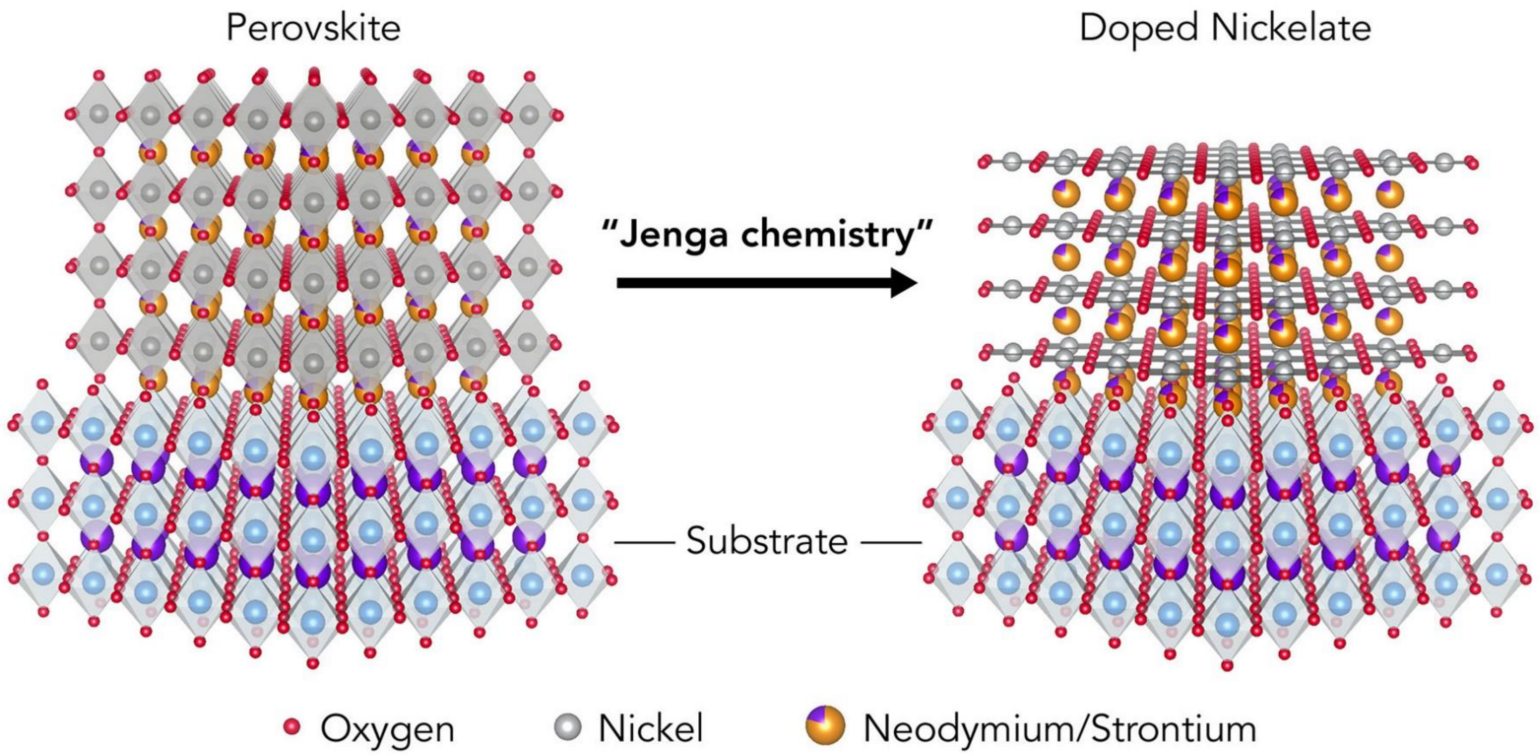
Comparaison Cuprates/Nickelates (Ni+)

Philippe Bourges – LLB/CEA Saclay



D. Li et al, Nature 572 624 (2019)

Theories Connected with High T_c Superconductivity

1. Resonating valence bonds
2. Spin fluctuations
3. Stripes
4. Anisotropic phonons
5. Bipolarons
6. Excitons
7. Kinetic Energy lowering
8. d-density wave
9. Charge fluctuations
10. Loop currents
11. Gossamer superconductivity
12. Spin bags
13. SO(5)
14. BCS/BEC crossover
15. Plasmons
16. Spin liquids

Not to Mention

Interlayer tunneling

Marginal Fermi liquid

van Hove singularities

Quantum critical points

Anyon superconductivity

Slave bosons

Dynamical mean field theory

Slide from Mike Norman (ANL) (2011)

+

CDW

SU(2)

Intertwinned orders

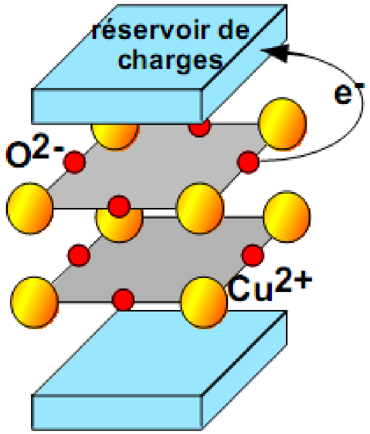
High Tc cuprates : layered structure

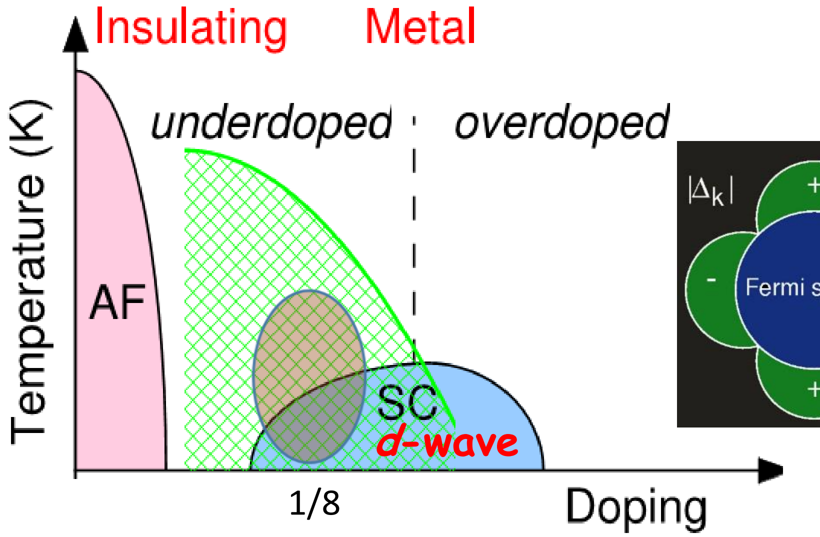
$HgBa_2CuO_{4+x}$
$(Nd,Pr)_{2-x}Ce_xCuO_4$

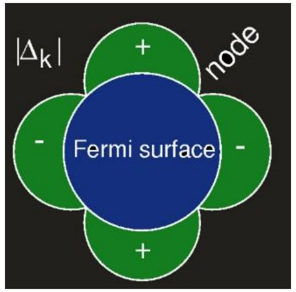
$La_{2-x}Sr_xCuO_4$
$YBa_2Cu_3O_{6+x}$

$Bi_2Sr_2CaCu_2O_{8+\delta}$
$Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$

$Tl_2Ba_2CuO_{6+\delta}$







- All interesting physics embebded in CuO layers
- Cu spins : antiferromagnetic correlations
  1 band Hubbard model, t-J model, RVB state…

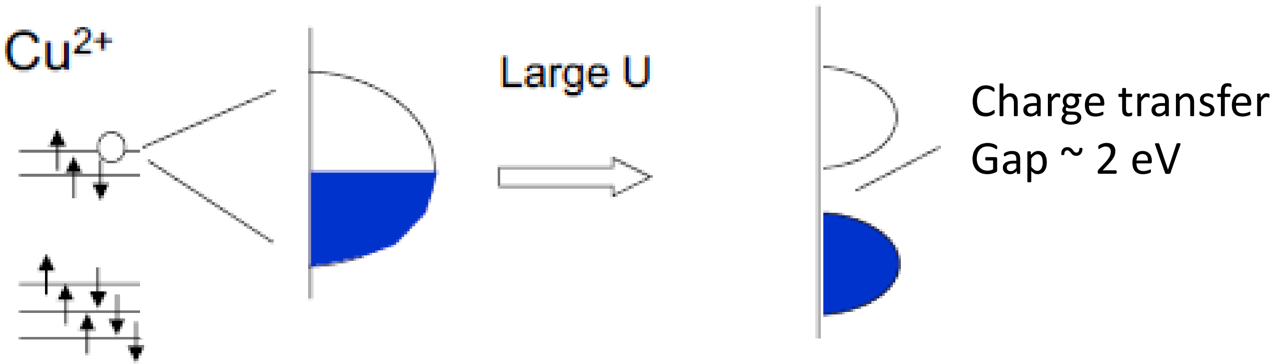
Common believe

Interactions

- Charge segragation (1D stripes/electronic nematic order)
- Nature of pseudogap below T* (underdoped state)
- Hidden order parameter: Spin order, Charge order,
  more exotic: loop current, D-Density Wave,…
- Since 2011: Charge Density Wave (NMR, resonant and hard xrays,…)
  (maximum around 1/8 doping)

Strong Electronic Correlations

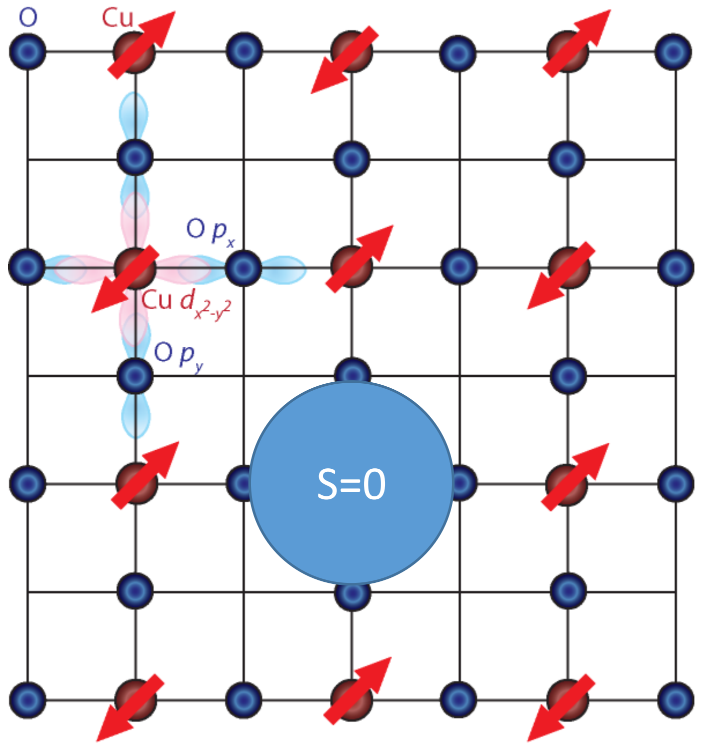
Cuprates: strongly correlated electronic system



$3d^9$ Cu^{2+}, dx^2-y^2, Spin S=1/2, AFM insulator

$$H = -t \sum_{i,j,\sigma} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$ Hubbard

$t = 0.3$ eV, $U = 2$ eV, $J = 4t^2/U = 0.12$ eV



Hole doping: Zhang-Rice singlet

Charge inhomogeneities, 1D stripes

Is it enough ?

- Electron phonon coupling
- Include oxygen orbitals (3 bands model)

Pseudogap below T* > Tc

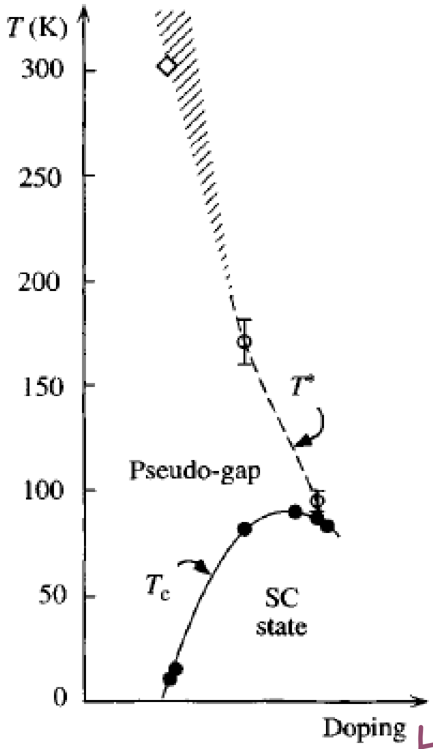
(In all physical properties)

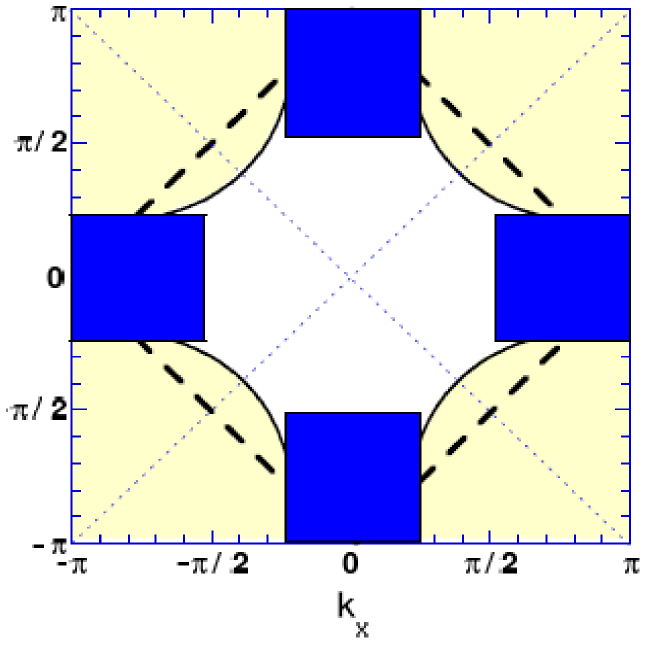
Hole and electron pockets:
p → 1+p   (Hall number)

ARPES/STM:

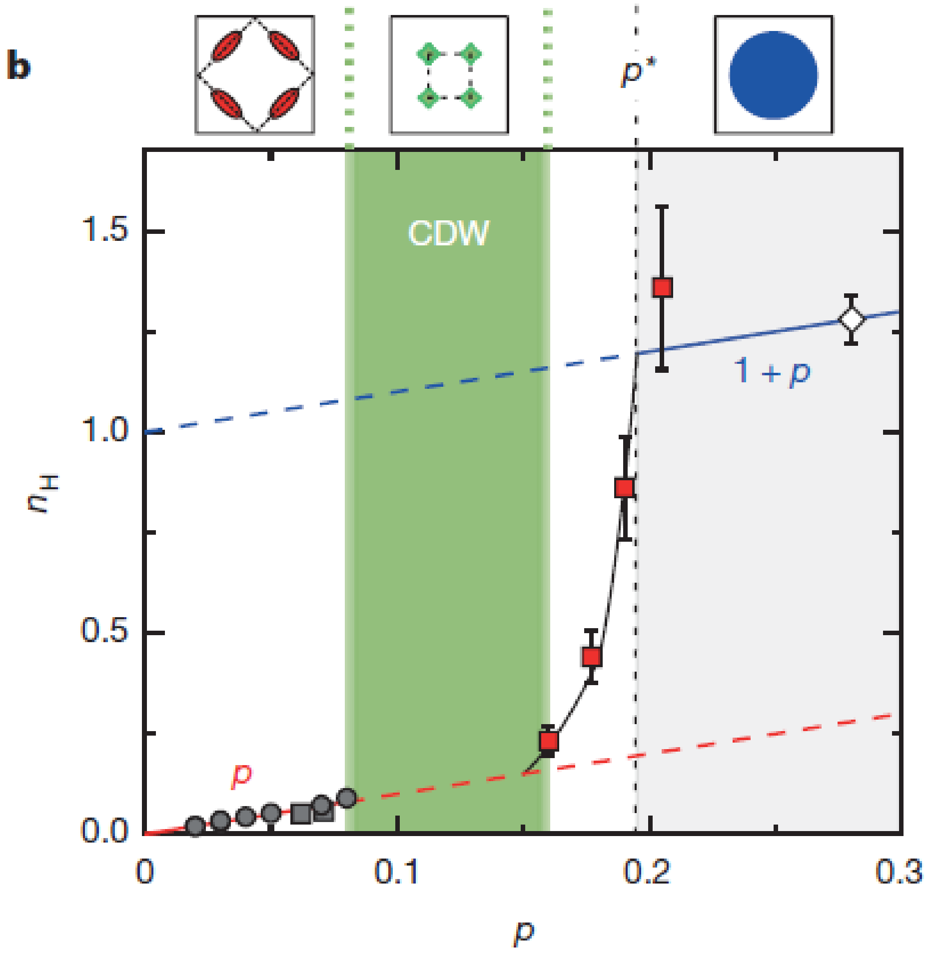
- 2D Fermi surface → t' ≈ -0.3 t
- Pseudogap state T < T*

« missing states » Fermi arcs





H. Ding et al, Nature 382 51 (1996)



S. Badoux et al, Nature 531 210 (2016)

Pseudo -gap: Hidden Ordered State

- Mysterious phase which appears below T*
- Anomalous magnetic and charge properties

→ Common line at T*

(Tallon & Loram)

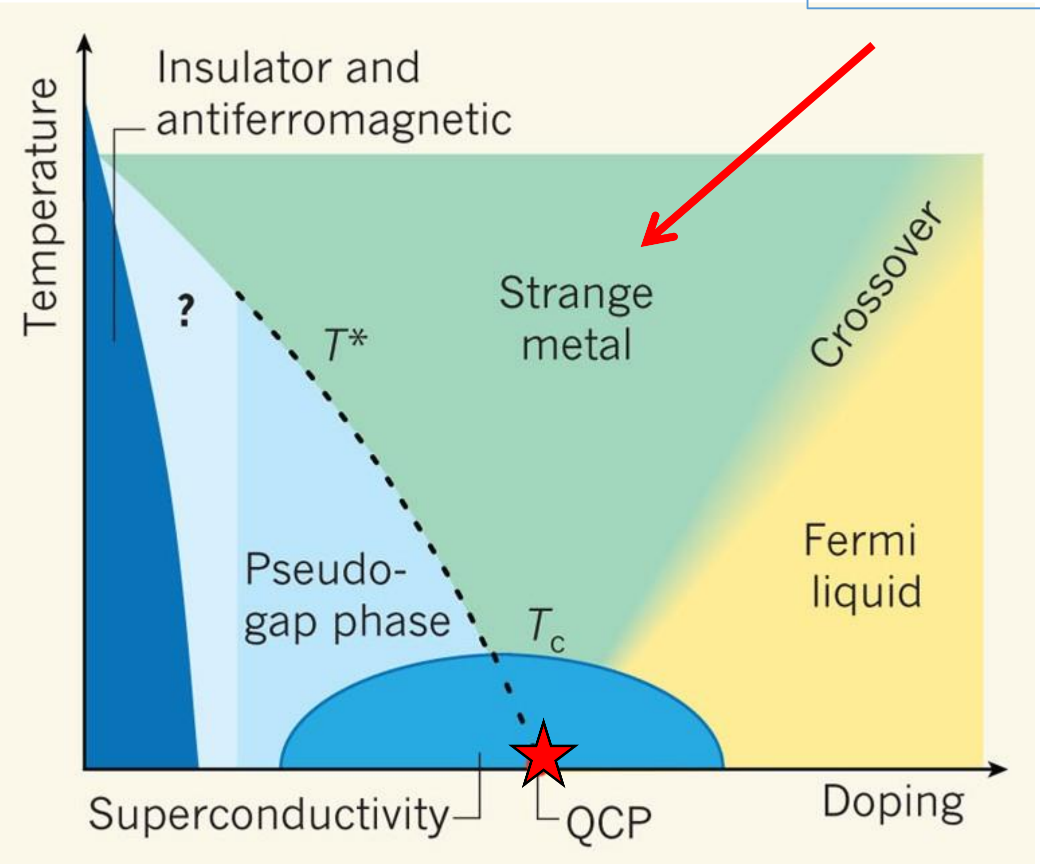
No sharp thermodynamic anomaly ➔ Crossover

Elec. phase transition ?

Which broken symmetry ?

Heavy fluctuations around QCP
Superconducting mechanism?

Bad metal:
mean free path ~ a
Resistivity ~ T



Quantum critical point

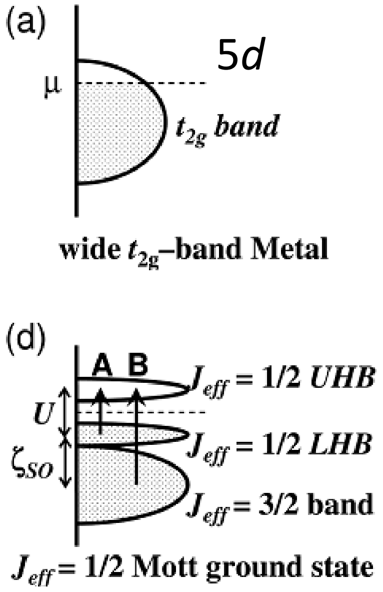
Broken Time reversal and inversion symmetries → Loop currents (Varma)

Iridates: Spin-orbit coupled Mott insulator

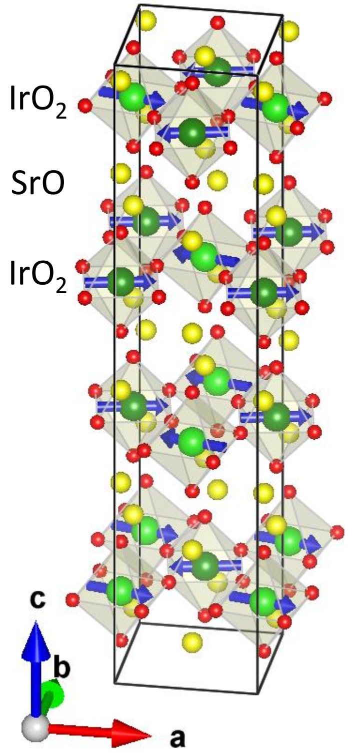
Strong Coulomb repulsion and spin-orbit coupling cause the Mott insulating state and J_{eff}=1/2 Heisenberg AFM on Ir sites.

Pseudogap
No superconductivity

Sr_2IrO_4



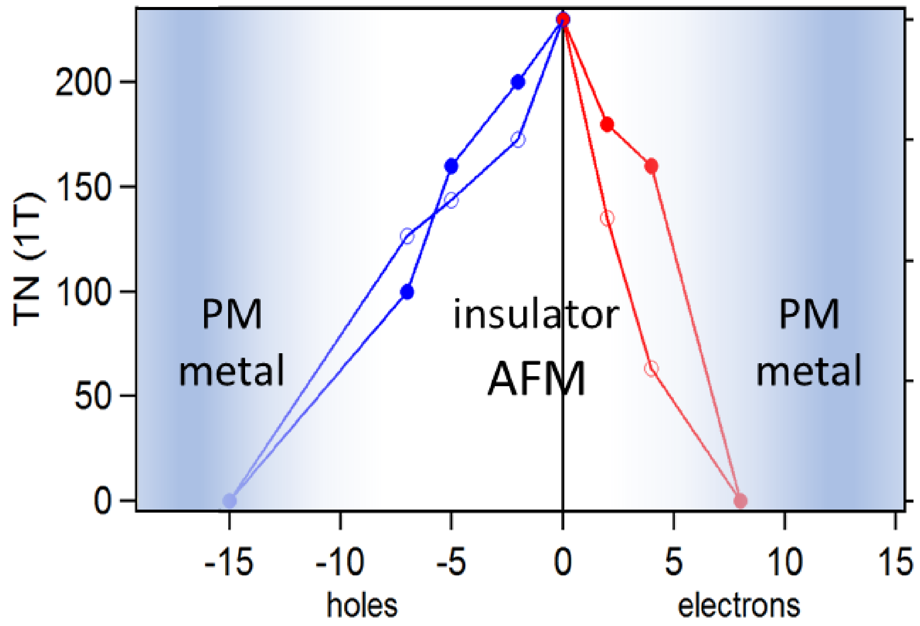
Layered perovskite
In-plane canted AFM



B. J. Kim *et al.*, PRL **101**, 076402 (2008)
B. J. Kim *et al.*, Science **323**, 1329 (2009)

Hole-doping $Sr_2(Ir,Rh)O_4$

Electron-doping $(Sr,La)_2IrO_4$

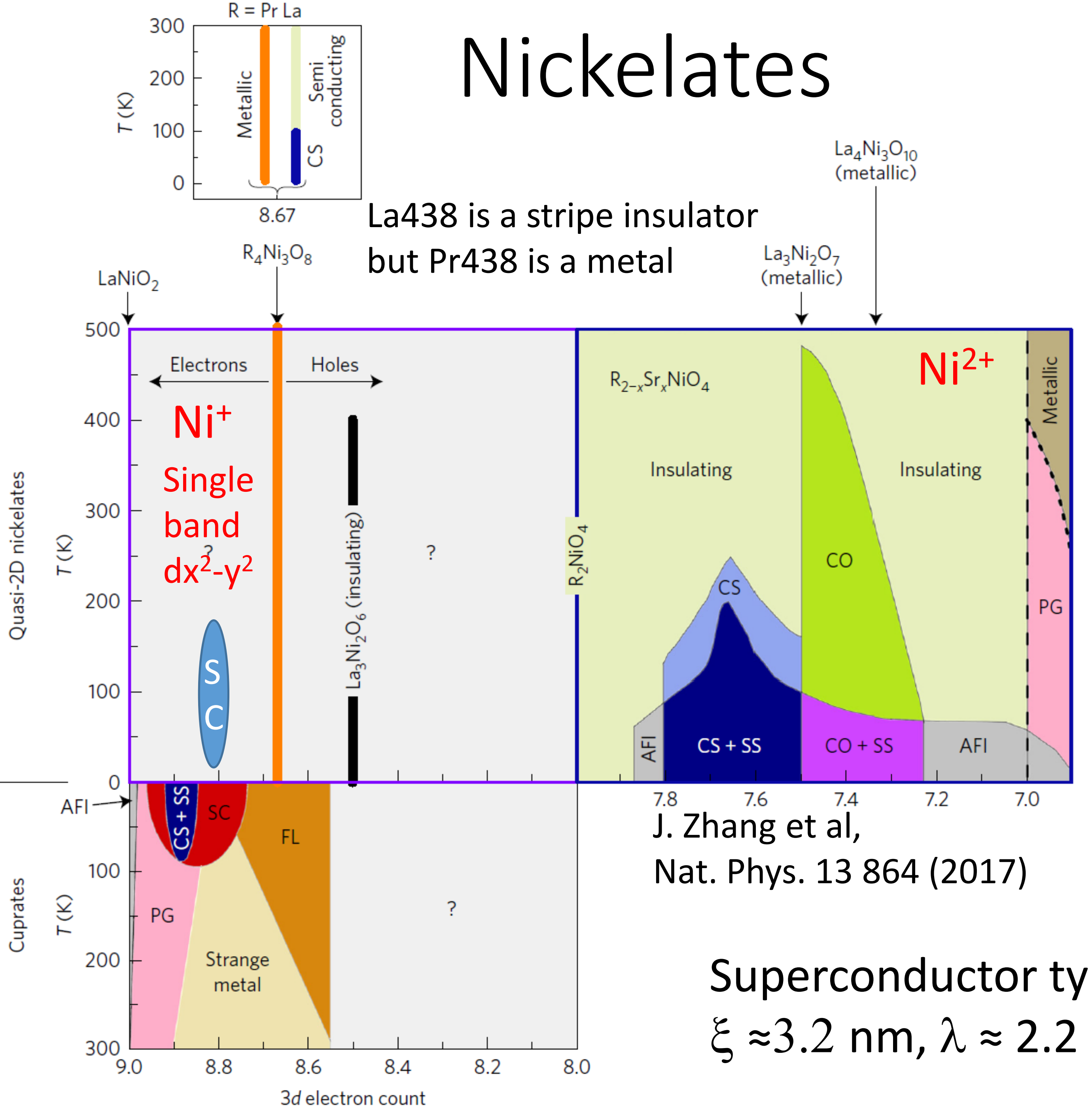


J. P. Clancy *et al.*, PRB **89**, 054409 (2014)
V. Brouet *et al.*, PRB **92**, 081117 (2015)
Y. Cao *et al.*, Nat. Commun. **7**, 11367 (2016)
A. de la Torre *et al.*, PRL **115**, 176402 (2015)

What is important in cuprates: for normal state & superconducting mecanism

- Layered structure → 2D physics
- Strong correlations vs weak correlations (FLEX)
- Mott physics (RVB, DMFT), Charge transfer insulating parent compound
- Role of magnetism ($3d^9$ Cu^{2+}, Spin S=1/2, AFM parent phase)
- Unconventionnal superconductivity: d-wave order parameter
- Stripes ordering and Charge order (or CDW)
- Electronic Inhomogeneities (STM, NMR,…)
- Band structure Topology (Fermi « arcs ») and Pseudogap
- Hidden orders, strange metal, Quantum Critical Point
- …

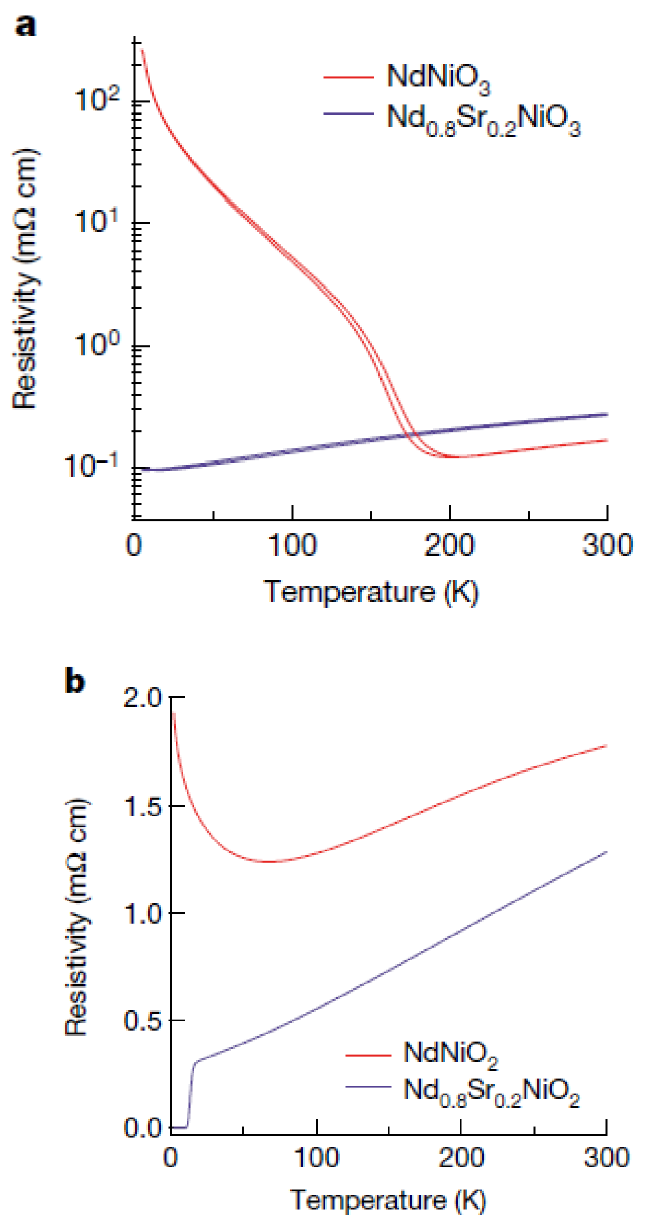
Nickelates



La438 is a stripe insulator
but Pr438 is a metal

J. Zhang et al,
Nat. Phys. 13 864 (2017)

D. Li et al, Nature 572 624 (2019)



Superconductor type II
$\xi \approx 3.2$ nm, $\lambda \approx 2.2$ μm

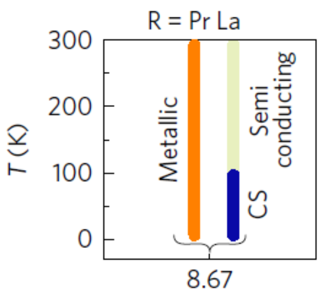
Nickelates

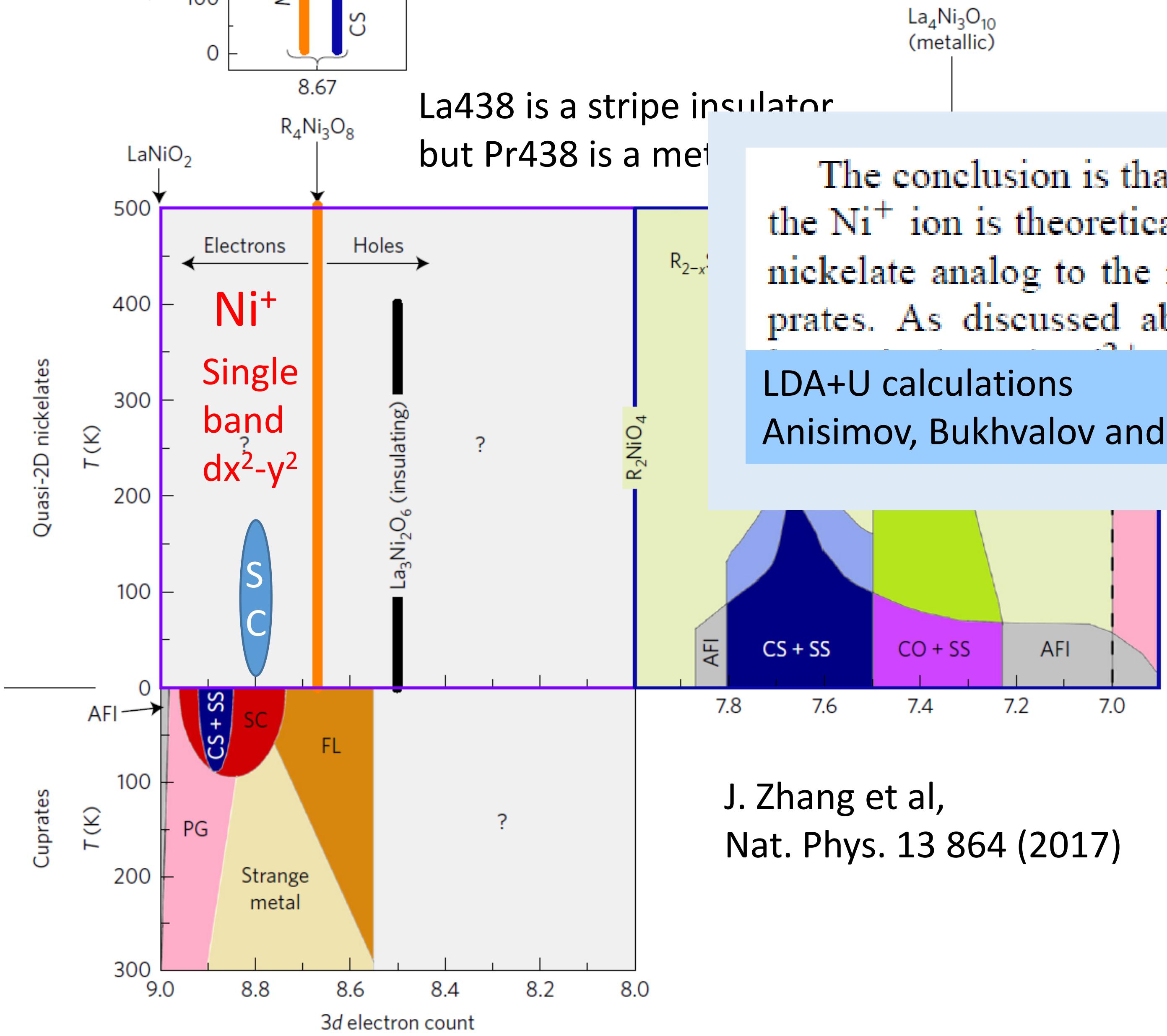
D. Li et al, Nature 572 624 (2019)

La438 is a stripe insulator
but Pr438 is a met

The conclusion is that a $S=\frac{1}{2}$ magnetic insulator based on the Ni^{+} ion is theoretically possible which would be a direct nickelate analog to the insulating parents of the high-T_c cuprates. As discussed above, hole doping should lead to a

LDA+U calculations
Anisimov, Bukhvalov and Rice PRB 59 7091 (1999)





J. Zhang et al,
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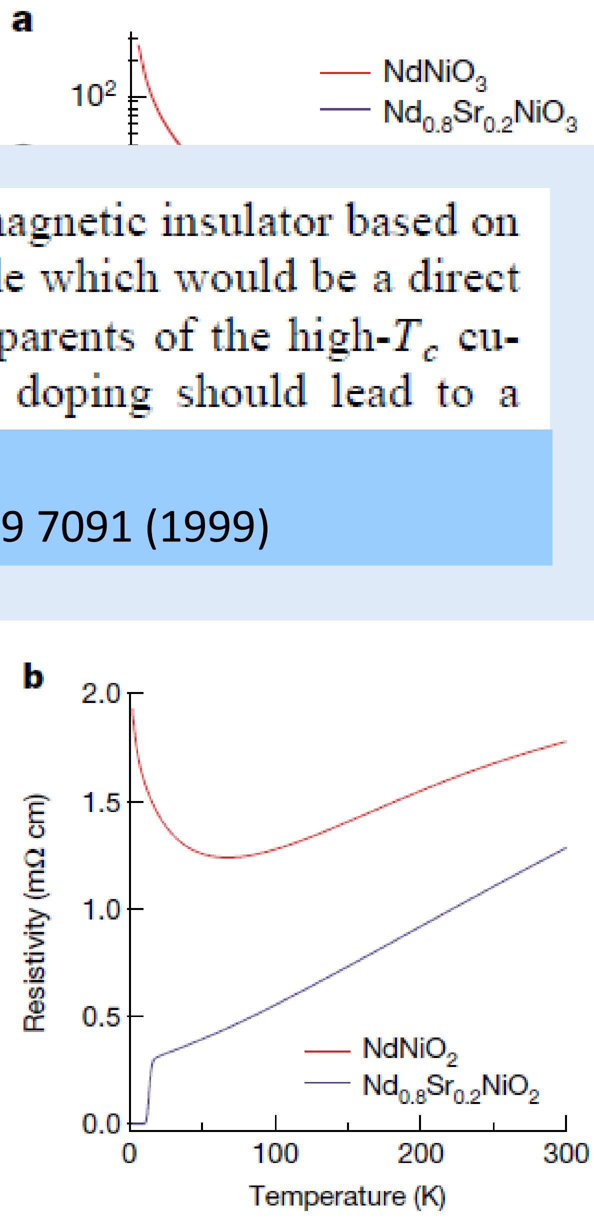
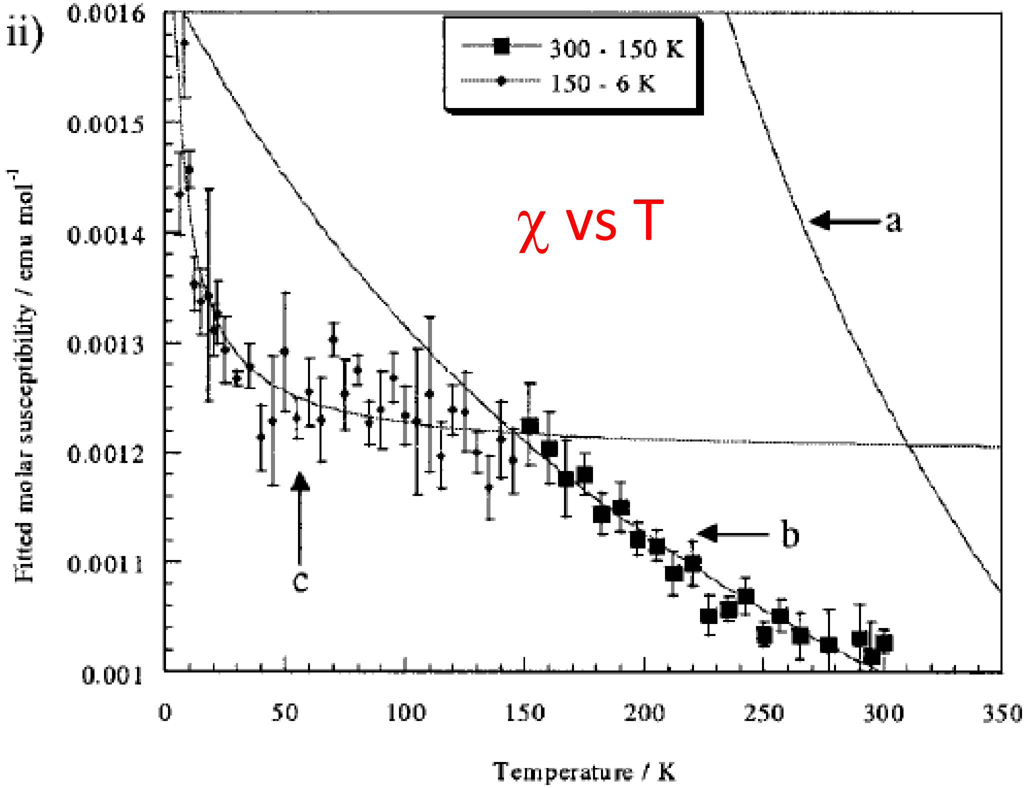


Magnetic measurements:

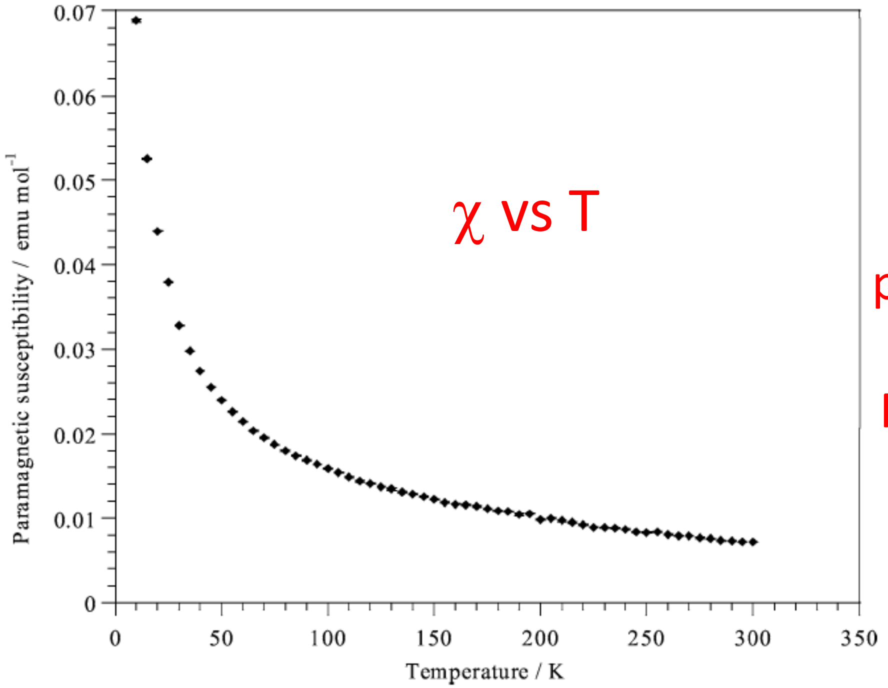
Unlike Cuprates and predictions, there is no evidence for magnetism in undoped materials.
Is it due to bad samples, Ni impurities, Nd moments,
self-doped holes, Kondo physics of mixed 5d Nd + 3d Ni ?

H. Zhang et al, 1909.07427 (2019)
G.M. Zhang et al, 1909.11845 (2019)

Powder neutron diffraction at 5 K (1.7 K), no AFM LRO (m < 0.05 (0.06) μB)



$LaNiO_2$: Hayward et al, JACS (1999)



No parent AFM Phase

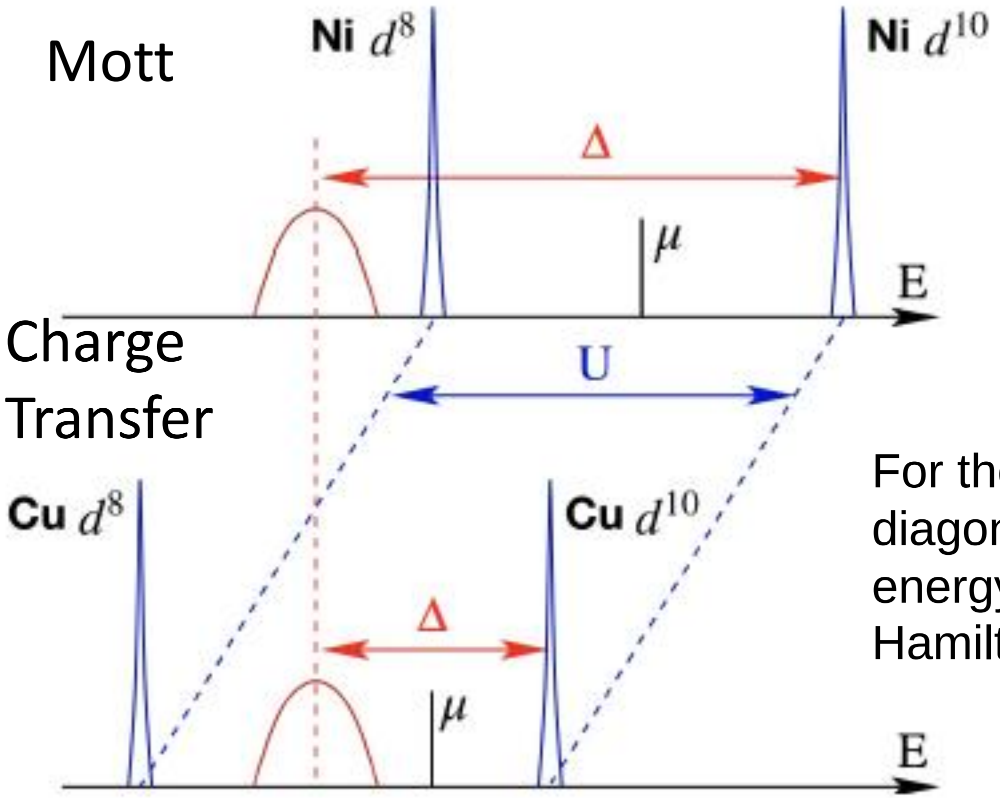
$NdNiO_{2.03}$: Hayward & Rosseinsky, SSS (2003)

Reduced spin fluctuations:

$$J_{dd} = \frac{4t_{pd}^4}{\Delta^2 U_{dd}} + \frac{8t_{pd}^4}{\Delta^2 (U_{pp} + 2\Delta)}$$

Mott

Charge Transfer



Jiang, Berciu & Sawatzky, 1909.02557 (2019)

Δ ~9 eV ($NdNiO_2$) to 3 eV (cuprates)

reduced but sizeable J ~13 meV

For the three-band Hubbard model, we perform the exact diagonalization studies of finite clusters Ni_5O_{16}, and map low-energy spectra onto the effective one-band t-t'-J model Hamiltonian with t = 260 meV, t' =-38 meV and J = 26 meV.

H. Zhang et al, 1909.07427 (2019)

Fermi surfaces:

Need ARPES !

Hall data seem to indicate small holes pockets for doped Phase and a large electron-like Fermi surface for the undoped phase

- Less O-Ni hydridization

- Doped holes primarily on the Ni Sites
  (unlike cuprates on oxygen)

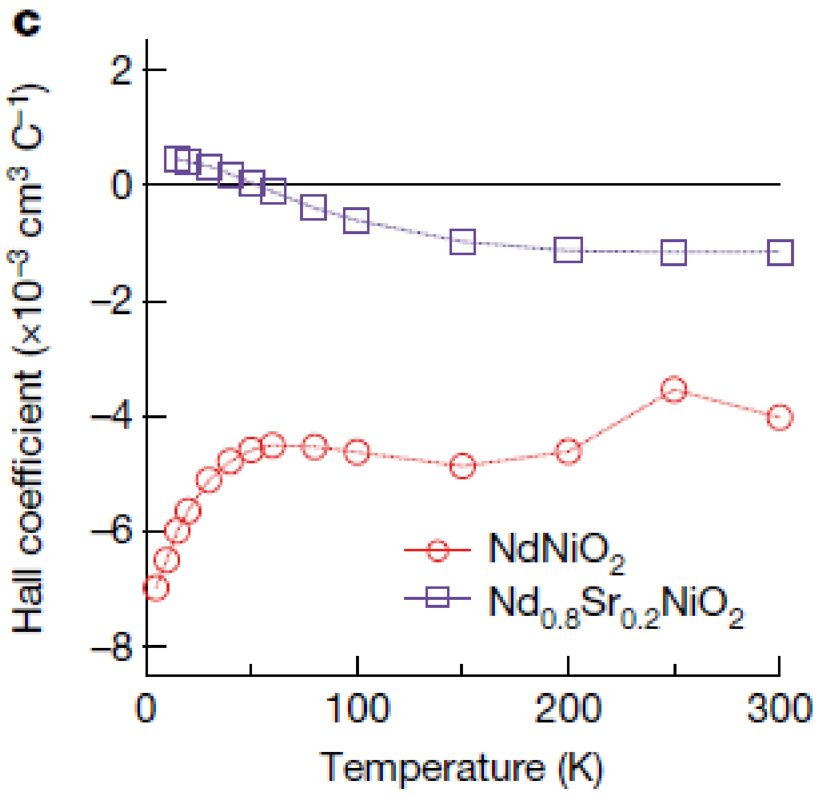
H. Zhang et al, 1909.07427 (2019)

(no Zhang-Rice singlet)

Kondo physics replaces the expected Mott insulator physics

Unlike cuprates with insulating spacer layers between the CuO_2 planes, the rare-earth spacer layer in the infinite-layer nickelate supports a weakly-interacting three-dimensional *5d* metallic state. This three-dimensional metallic state hybridizes with a quasi-two-dimensional, strongly correlated state with $3d_{x2-y2}$ symmetry in the NiO_2 layers.

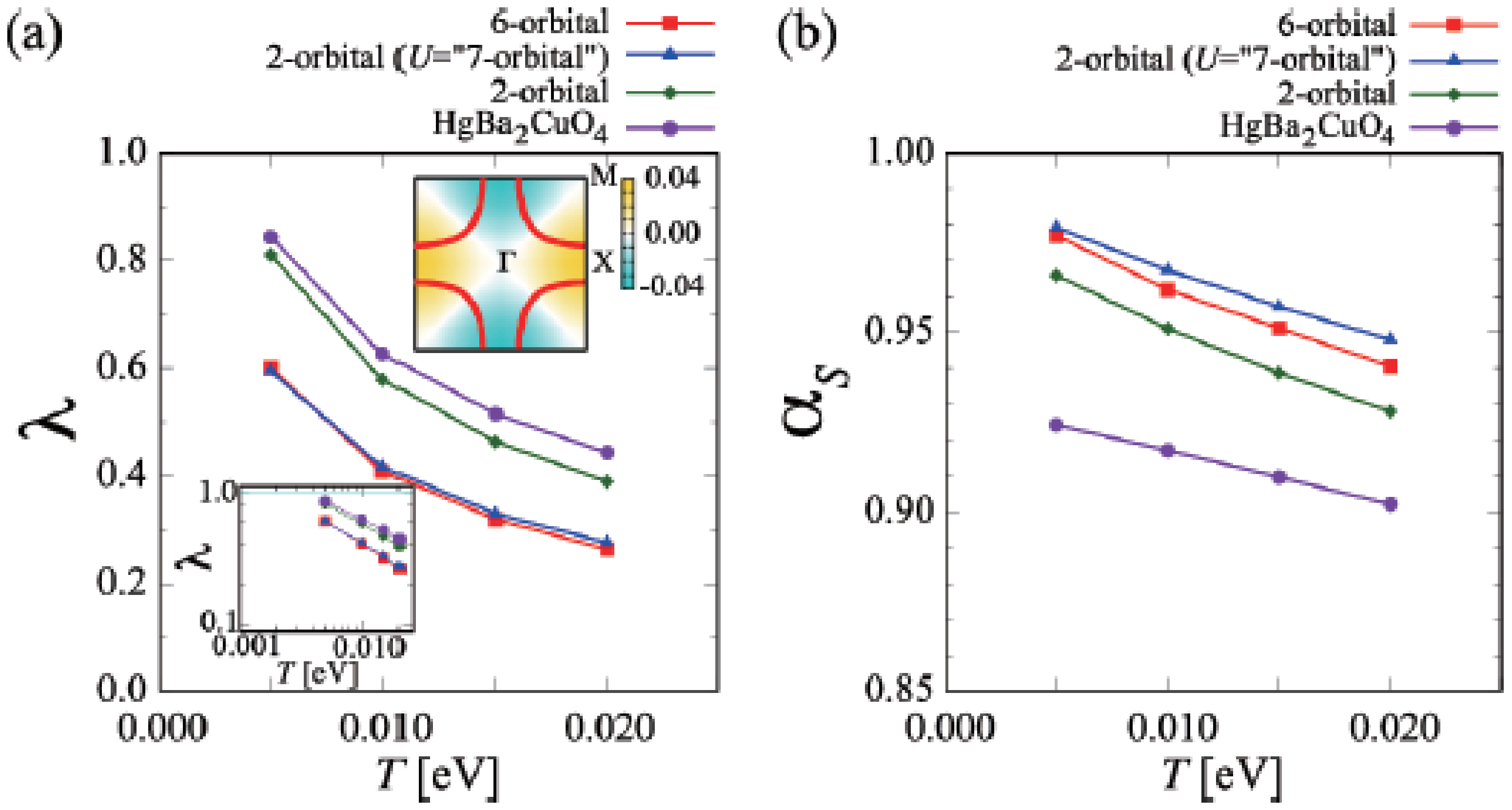
Hepting et al, 1909.02678 (2019)



D. Li et al, Nature 572 624 (2019)

Superconducting mecanism:

Spin fluctuations (AFM)
FLEX method: dx^2-y^2 order parameter



Interactions (α_S) relatively larger for Ni because of reduced bandwidth (this enhances competing order and reduces superconductivity)

Sakakibara et al 1909.00060 (2019)

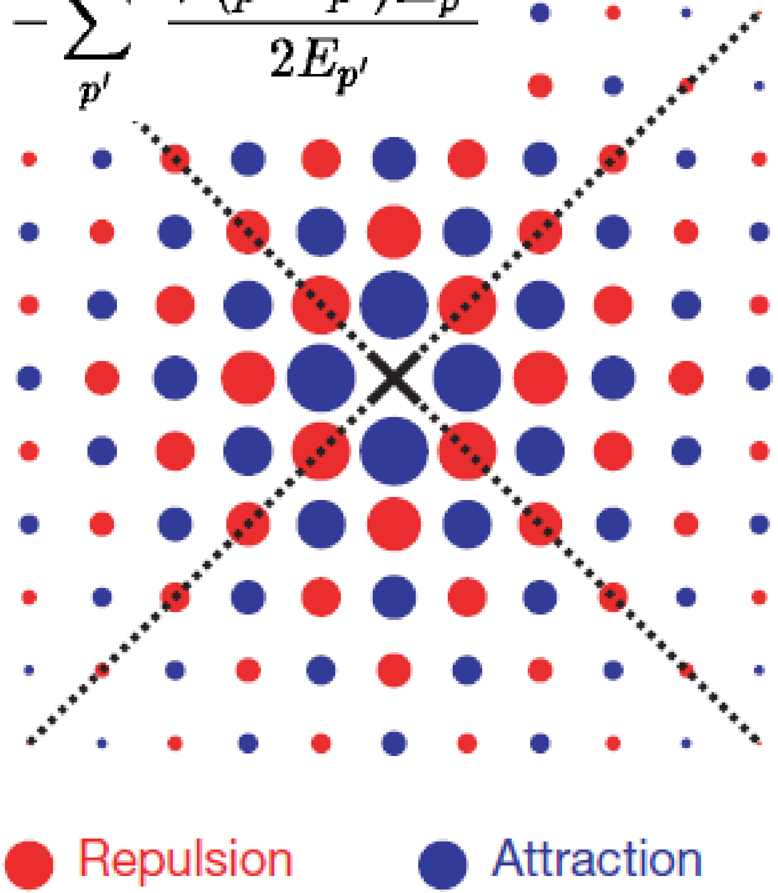
Similar conclusions from Hubbard RPA/t-J models X. Wu et al, 1909.03015 (2019)

Superconductivity without phonons

P. Monthoux, D. Pines & G. G. Lonzarich,

Spin fluctuations → d-wave SC

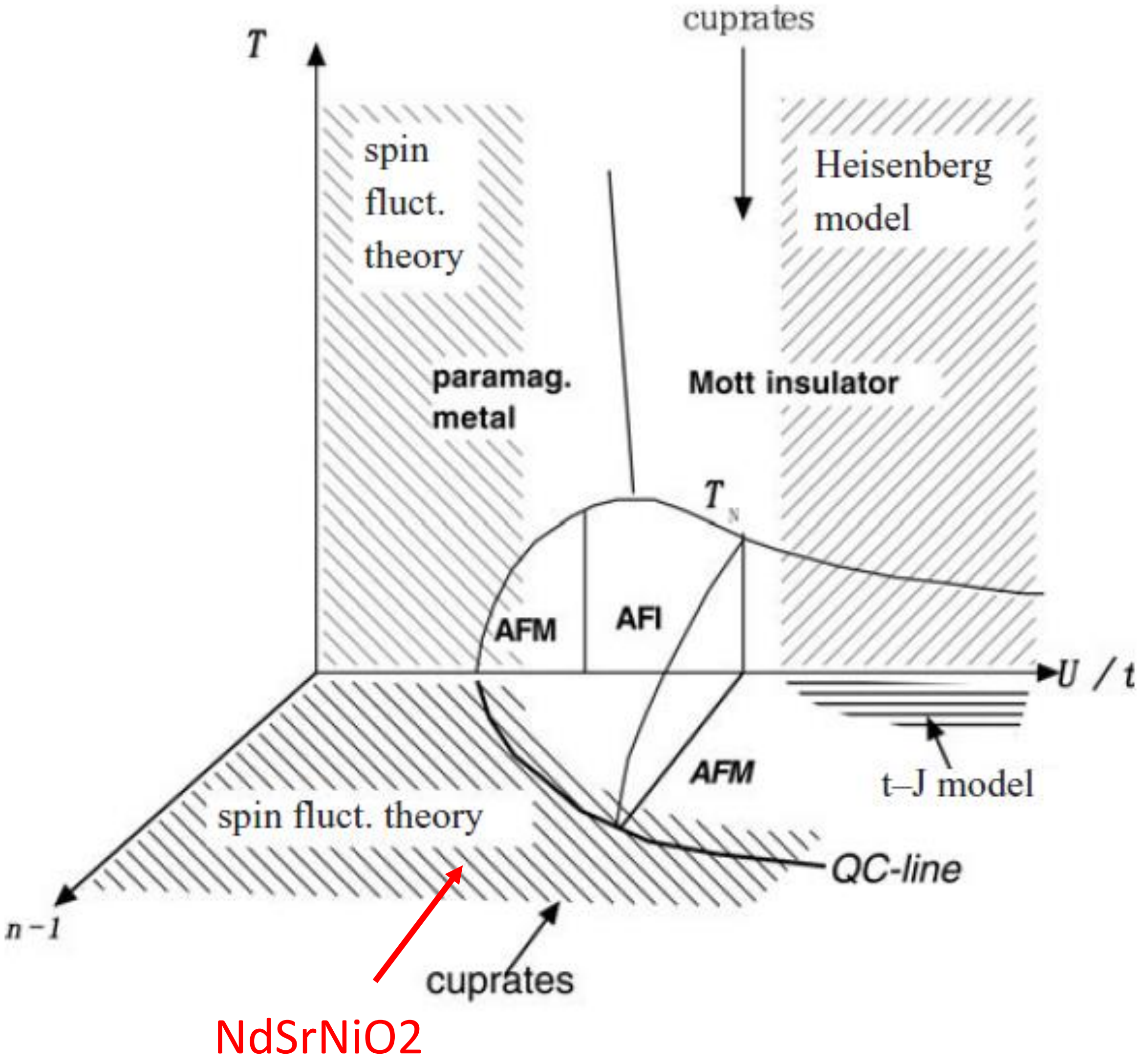
$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$



Magnetic interaction potential in AFM lattice

Antiferromagnetic spin fluctuation and superconductivity

Moriya & Ueda 2003 *Rep. Prog. Phys.* **66** 1299



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?

What to do ?

- Grow bulk and single crystals
- Map the phase diagram (hole and electron doped).
- ARPES (band structure)
- Measure Spin fluctuations: NMR, μSR, Inelastic neutron, RIXS ??
- Measure superconducting gap (ARPES, …).