Nickelate superconductivity

Quick review and open questions

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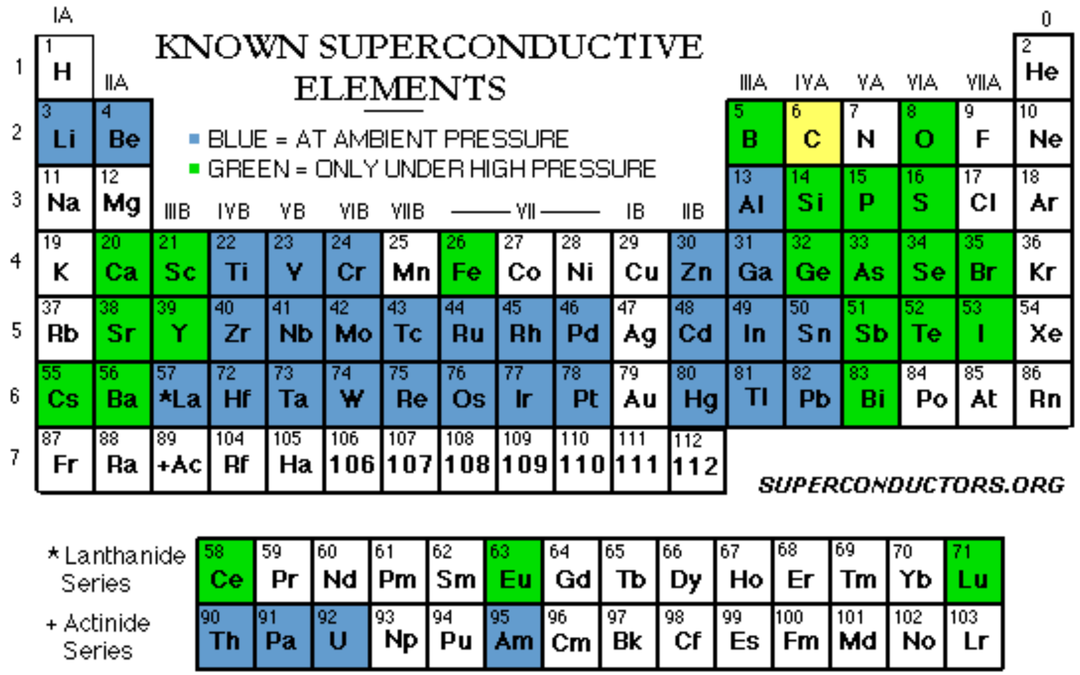
Finding a new superconductor



BCS, Type-I, “conventional” recipe:

- Get an elemental metal
- Compress to GPa if necessary
- For the best metals, get better cryogenics, e.g. lithium, T_c = 0.4 mK

  J. Tuoriniemi et al, Nature 447 (2007)

- Don’t use magnetic metals

Finding a new superconductor

Heavy fermions $CeCu_2Si_2$, $U_{1-x}Th_xBe_{13}$, $CeIn_3$, $CeRhIn_{5,...}$

Cuprates $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+\delta}$, $HgBa_2Ca_2Cu_3O_{9,...}$

Organics $(TMTSF)_2M$ (M = PF_6, SbF_6, ReO_4), $(BEDT\text{-}TTF)_2M$,…

Magnetic UGe_2, Sr_2RuO_4, $ZrZn_{2,...}$

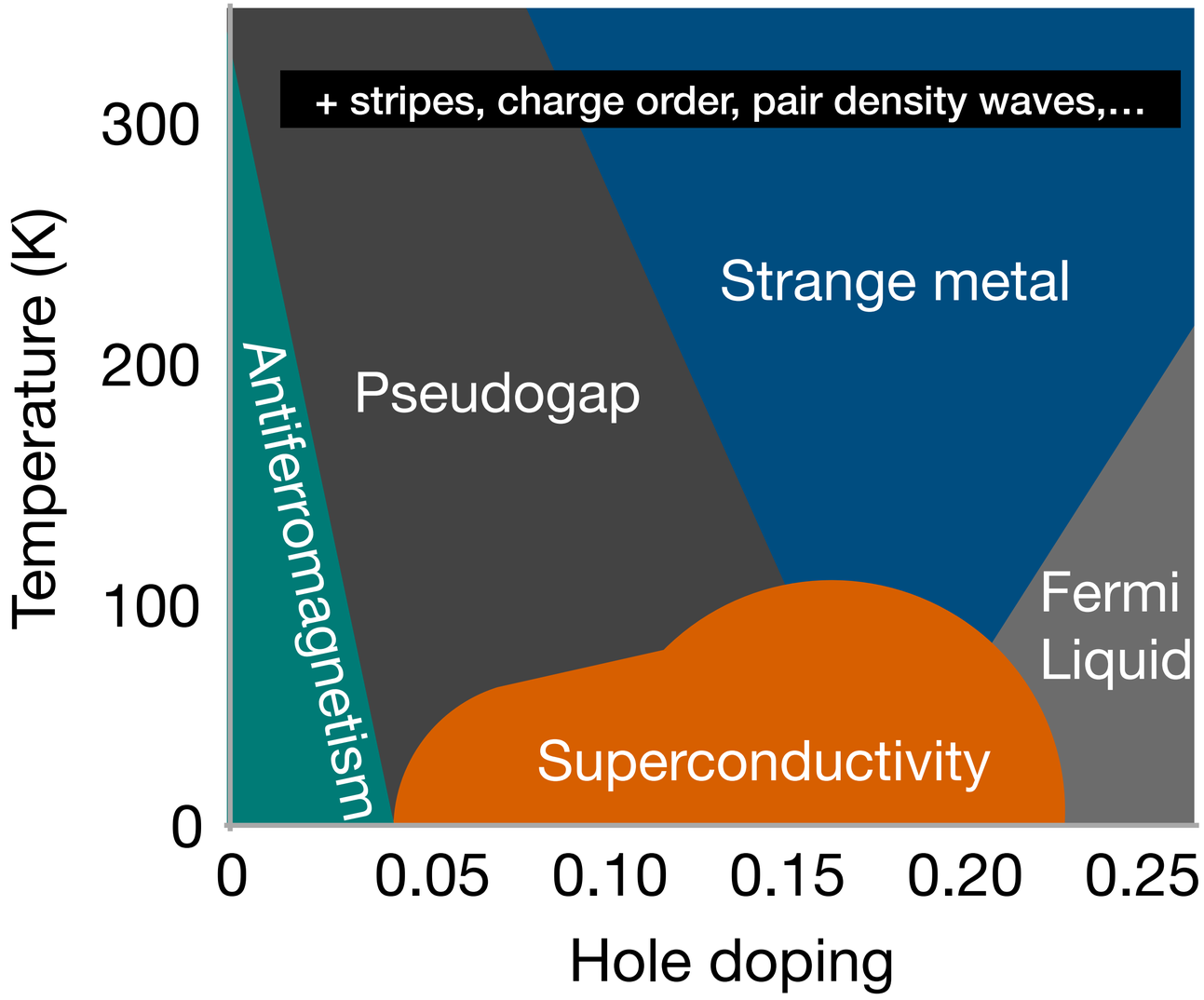
Pressurized $Na_{0.3}CoO_2(H_2O)_{1.4,...}$

Others $PuCoGa_5$, $PrOs_4Sb_{12}$, $CaPt_3Si$, UIr, Li_2Pt_3B, $LaAlO_3/SrTiO_3$, ZrNCl, FeAs, NbN, NbC, magic angle graphene, twisted WSe_2, K_3C_{60},…

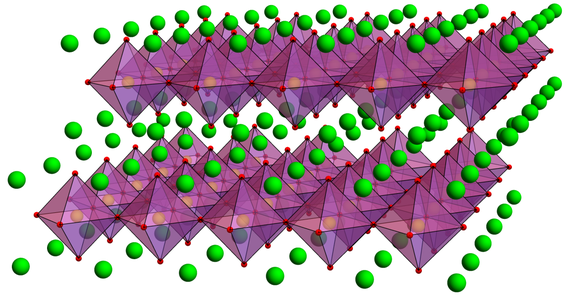
non-BCS, “unconventional” recipe:

- Get metallicity
  - Compress to GPa if necessary
  - Cool down more if necessary
  - Improve sample quality
  - Cross fingers

High temperature superconducting copper oxides



Adapted from B. Keimer et al, Nature 518 (2015)

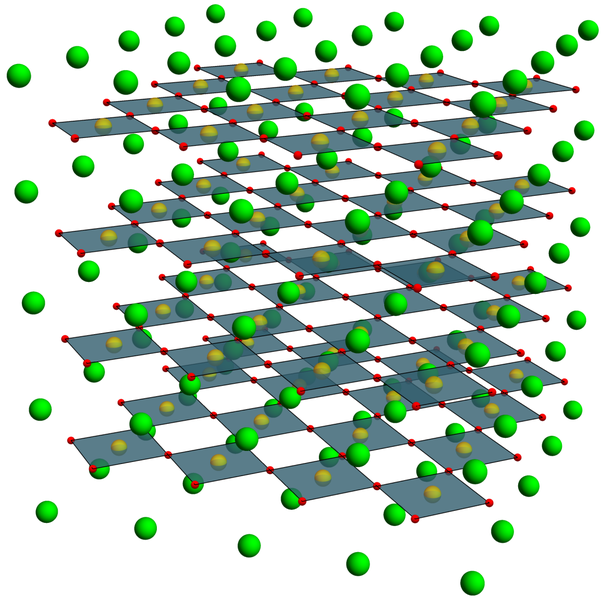


e.g. La_2CuO_4 with Sr dopants

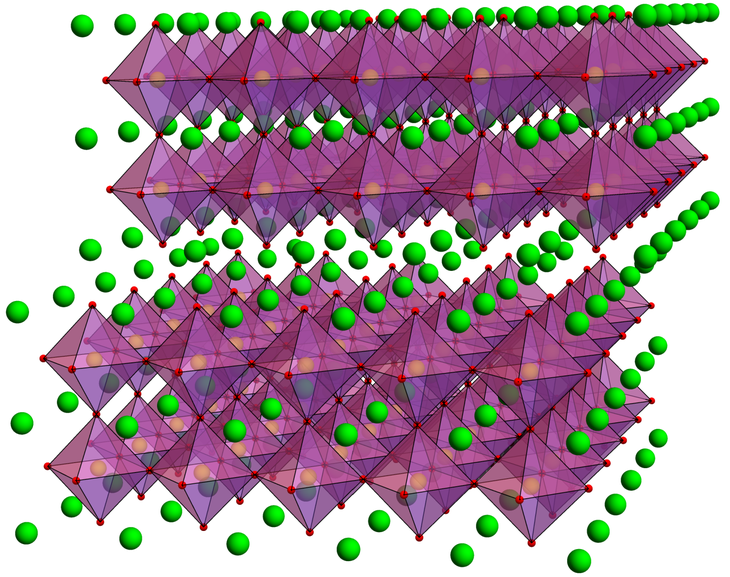
Recipe:

- Quasi-2-Dimensional
- $3d^9$, Single hole in dx^2-y^2 orbital
- Antiferromagnetic correlations
- Strong TM *3d* - O *2p* hybridization

Nickelate superconductors

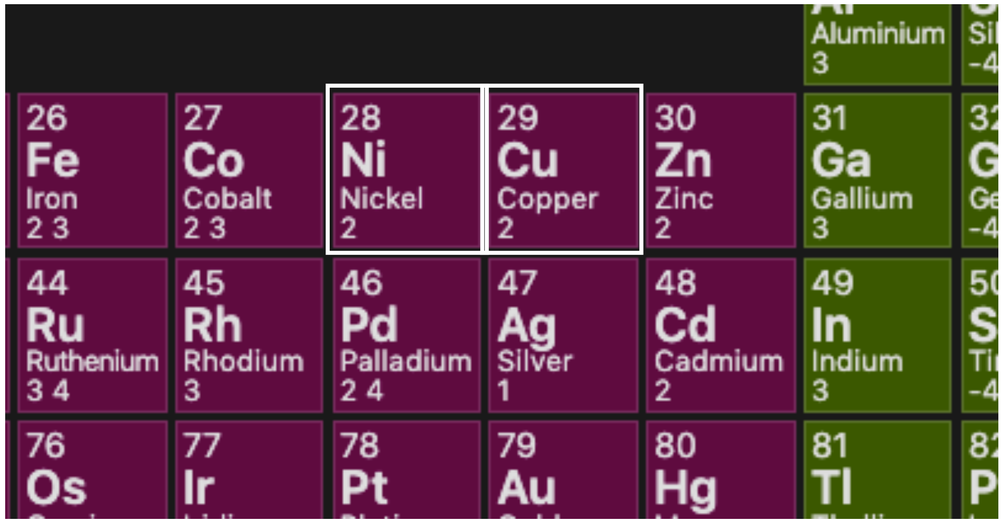


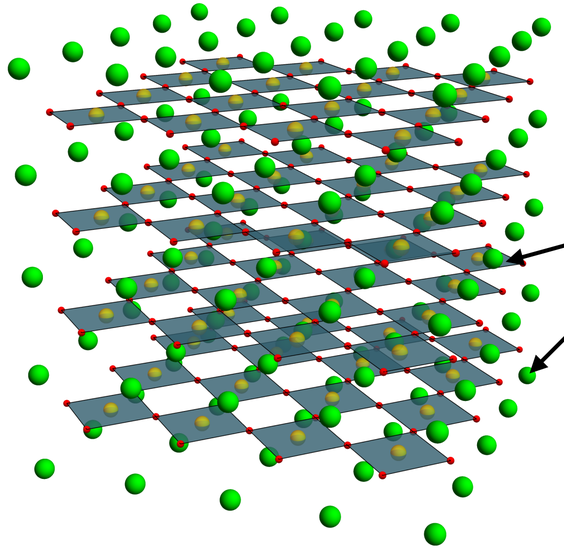
Square planar (2019)



Octahedral (2023)

Superconductivity in square-planar nickelates





"Infinite-layer" $RNiO_2$

NiO_2 square planar

Lanthanide

Ni^{1+} ($3d^9$)

V. I. Anisimov et al, Phys. Rev. B 59, 12 (1999)

"Electronic structure of possible nickelate analogs to the cuprates"

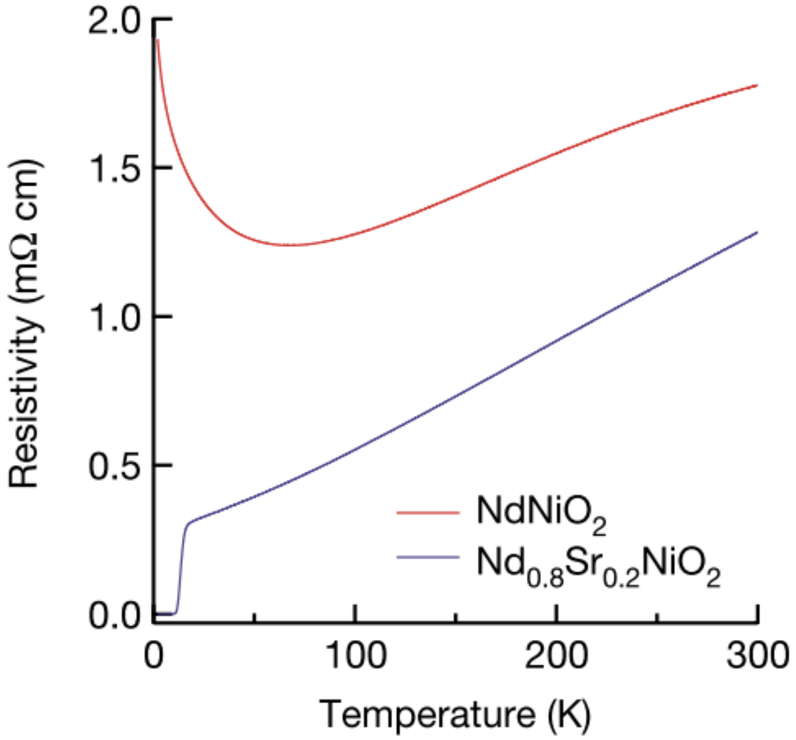
- Hole-doped square planar (e.g. infinite-layer) Ni^{1+} could be similar

K. W. Lee et al, Phys. Rev. B 70, 165109 (2004)

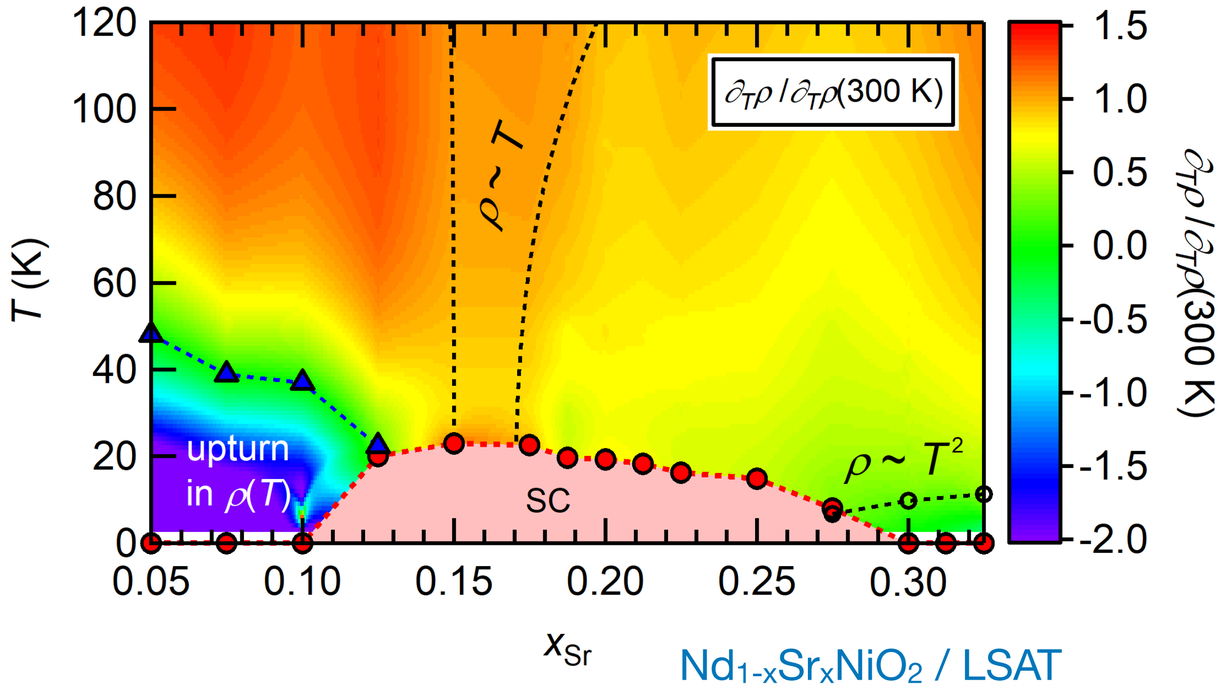
"Infinite-layer $LaNiO_2$: Ni^{1+} is not Cu^{2+}"

- Or not…?

Superconductivity in square-planar nickelates



D. Li et al, Nature 572 (2019)



$Nd_{1-x}Sr_xNiO_2$ / LSAT
Lee et al, Nature 619 (2023)

$Nd_{1-x}Sr_xNiO_2$
Li et al, Phys. Rev. Lett. 125 (2020)
Zeng et al, Phys. Rev. Lett. 125 (2020)

$Pr_{1-x}Sr_xNiO_2$
Osada et al, Nano Lett. 20 (2020)
Osada et al, Phys. Rev. Mater. 4 (2020)

$Nd_{1-x}Eu_xNiO_2$
W. Wei et al, Sci. Adv. 9 (2023)

$La_{1-x}A_xNiO_2$
Osada et al, Adv. Mater. 33 (2021)
Zeng et al, Sci. Adv. 8 (2022)

$Nd_6Ni_5O_{12}$
Pan et al, Nat. Mater. 21 (2021)

(Sm, Eu, Ca, Sr)NiO_2
Chow et al, arXiv 2410.00144

Synthesis of metastable Ni^{1+}

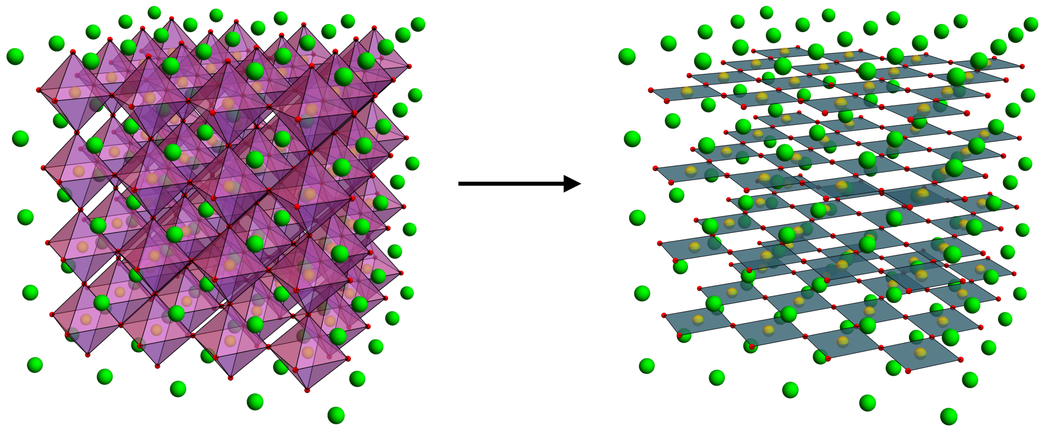
J. Chem. Soc., Faraday Trans. 2, 1983, **79**, 1181–1194

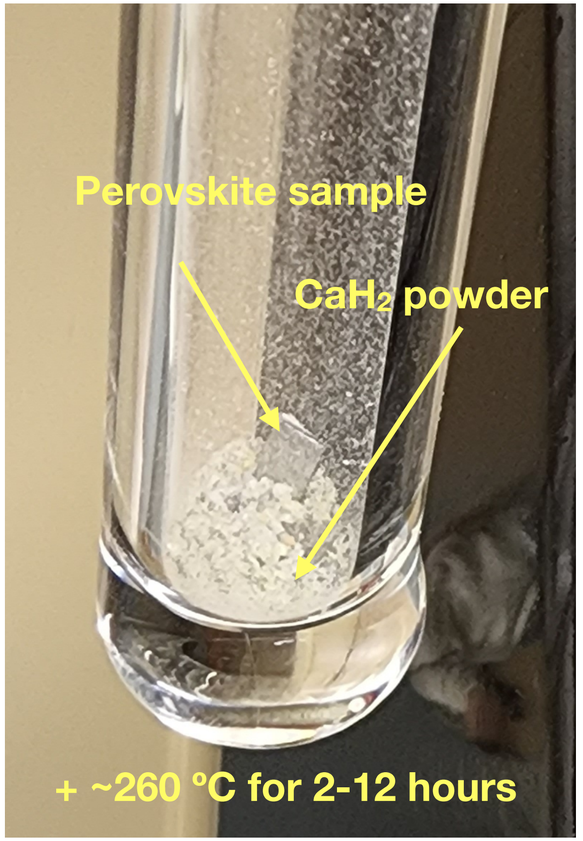
Reduced Forms of $LaNiO_3$ Perovskite

Part 1.—Evidence for New Phases: $La_2Ni_2O_5$ and $LaNiO_2$

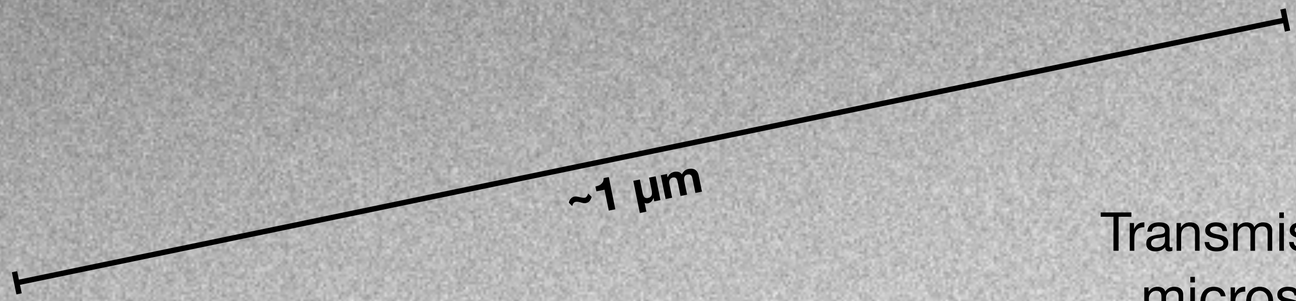
BY MICHEL CRESPIN, PIERRE LEVITZ AND LUCIEN GATINEAU*

Topotactic reduction by hydrogen gas



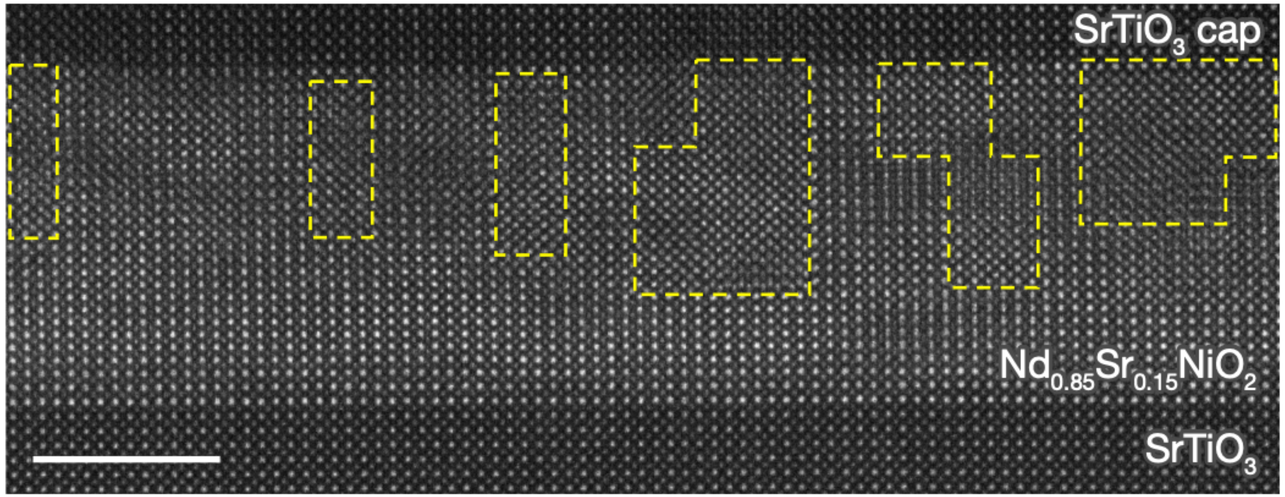


Superconductivity only observed in thin films



Transmission electron microscopy image courtesy of Berit Goodge, Cornell/MPI Dresden

Improving sample quality



Antiphase faults lead to worse superconductivity

Can be fixed by Ni-rich target, control of target history, imaging mode of the laser…

Lee et al, Nature 619 (2023)

Article

Critical role of hydrogen for superconductivity in nickelates

https://doi.org/10.1038/s41586-022-05657-2
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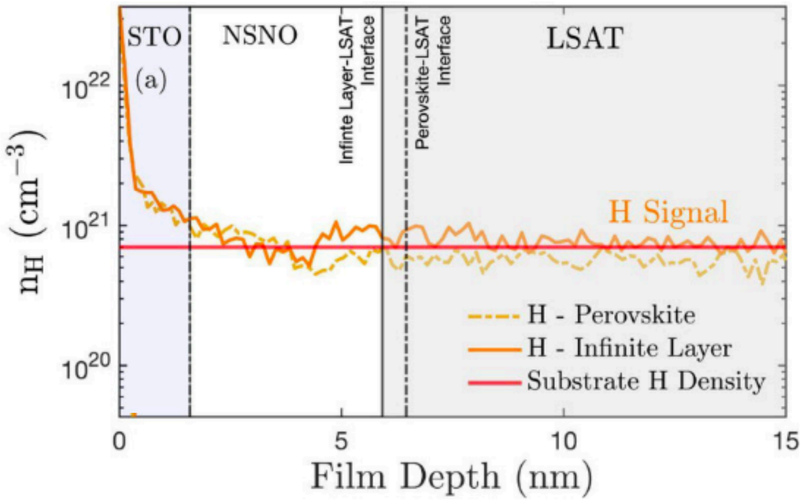
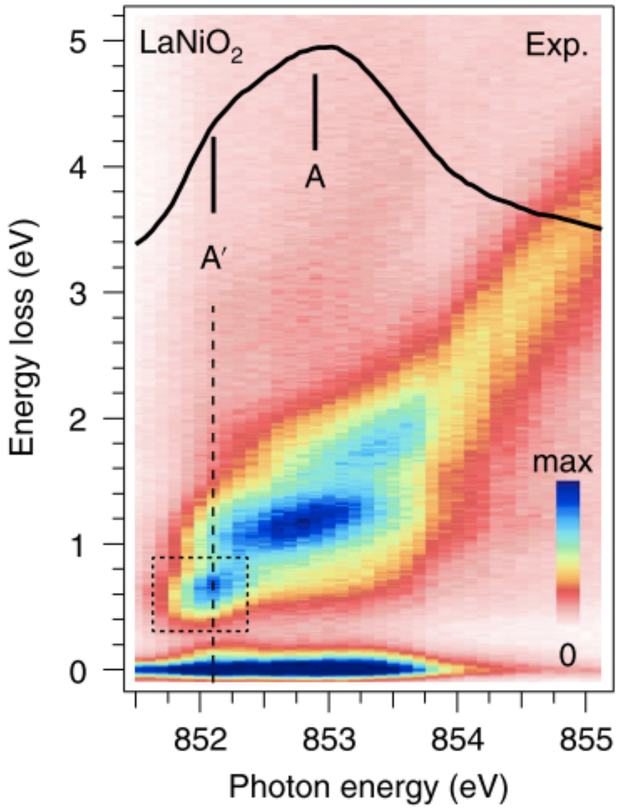
Xiang Ding[1,9], Charles C. Tam[2,3,9], Xuelei Sui[4,9], Yan Zhao[1], Minghui Xu[1], Jaewon Choi[2], Huaqian Leng[1], Ji Zhang[5], Mei Wu[6], Haiyan Xiao[1], Xiaotao Zu[1], Mirian Garcia-Fernandez[2], Stefano Agrestini[2], Xiaoqiang Wu[7], Qingyuan Wang[7]✉, Peng Gao[6], Sean Li[5], Bing Huang[4,8]✉, Ke-Jin Zhou[2]✉ & Liang Qiao[1]✉

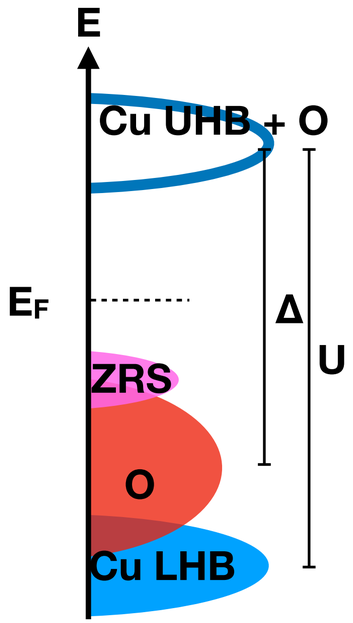


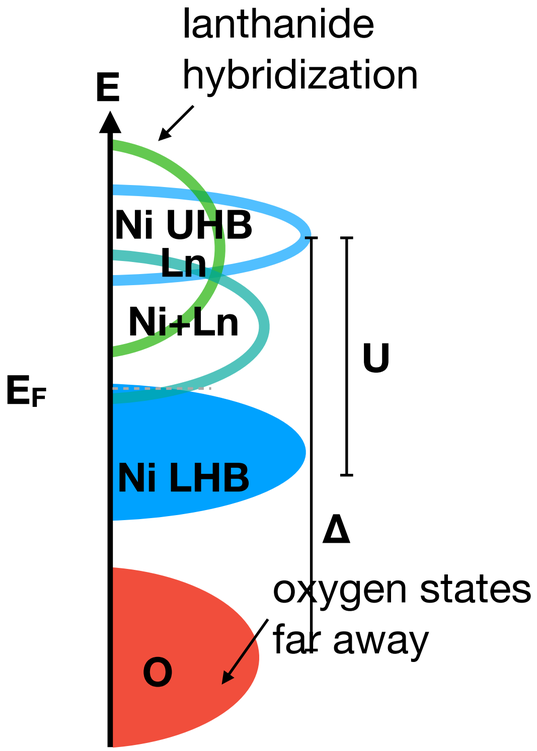
Secondary ion mass spectroscopy shows negligible hydrogen in good quality samples

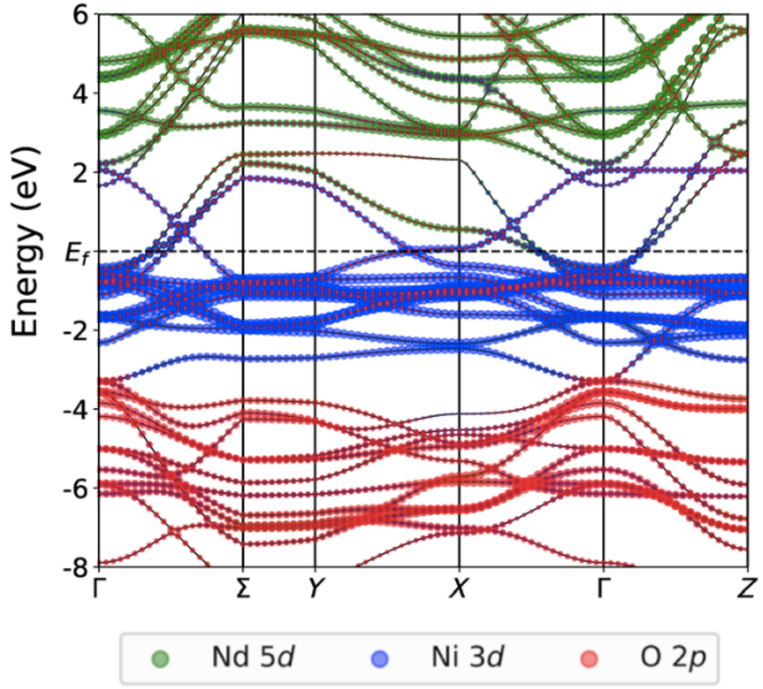
M. Gonzalez et al, Phys. Rev. Mater. 8 (2024)

Mott-hubbard character with lanthanide hybridization









Cuprates:
charge-transfer
physics

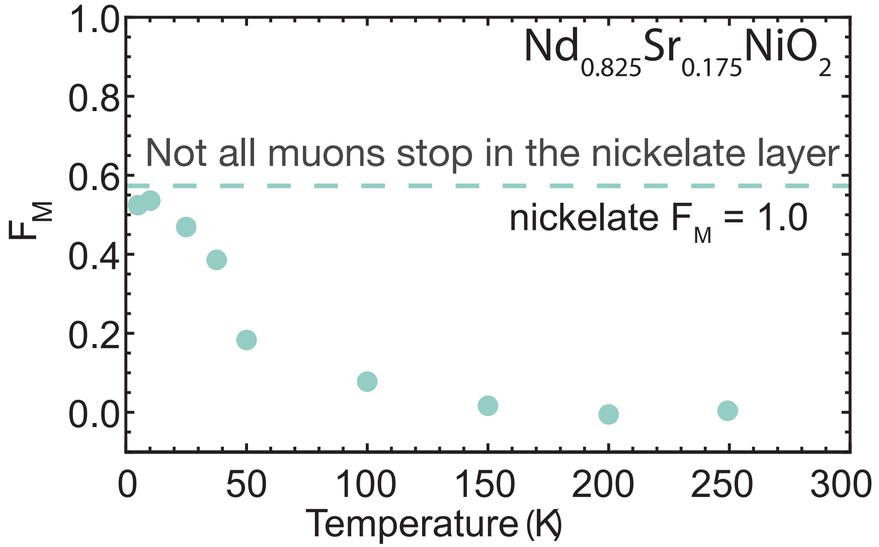
Nickelates:
more Mott-Hubbard-like
with lanthanide hybridization

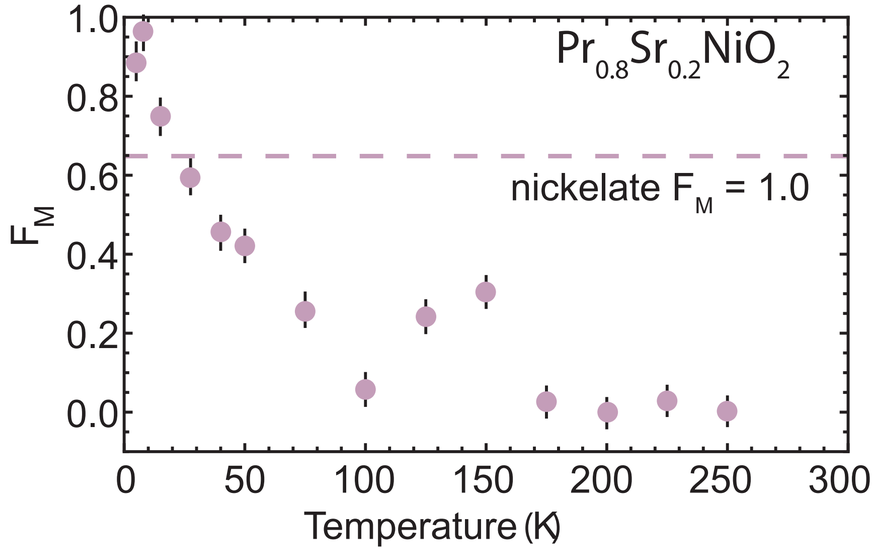
E. Been et al, Phys. Rev. X 11 (2021)
And many other *ab initio* works

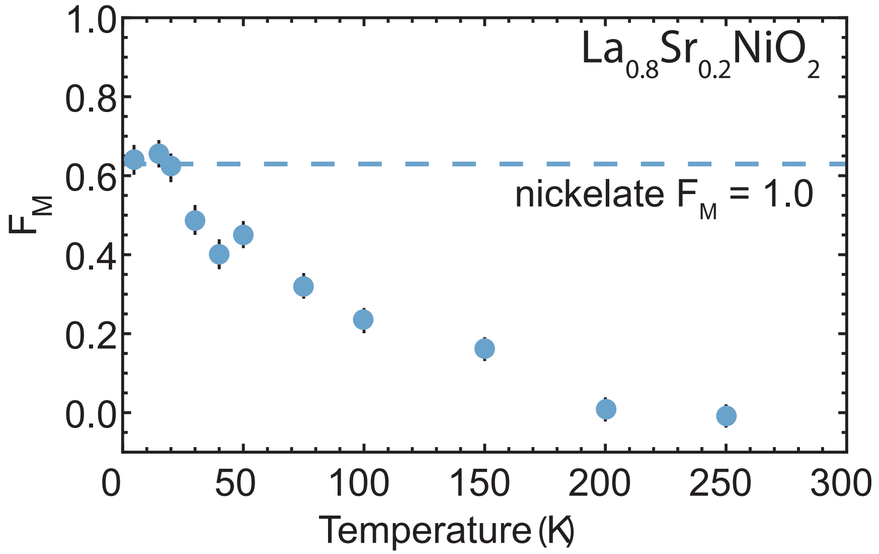
Resonant inelastic X-ray scattering
M. Hepting et al, Nat. Mater. 19 (2020)

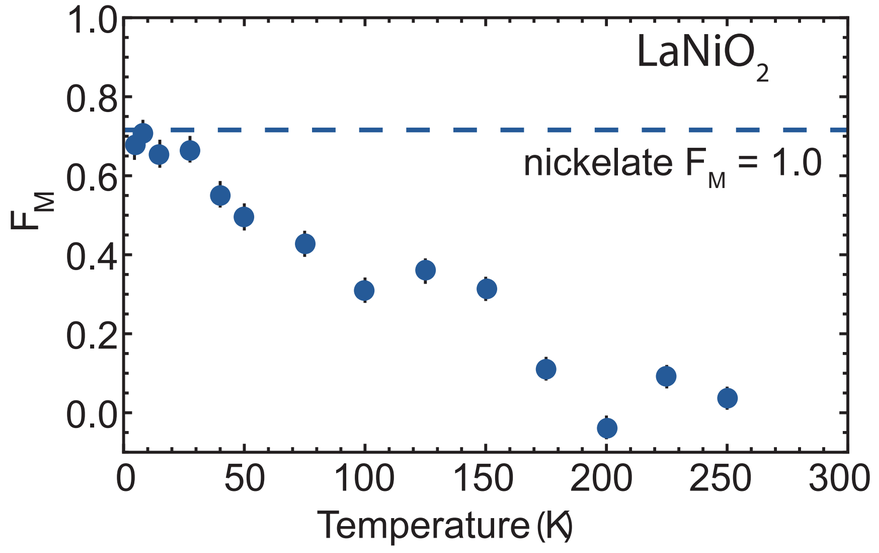
Superconducting square-planar nickelates are intrinsically magnetic

Magnetic volume fraction from weak transverse field muon spin rotation



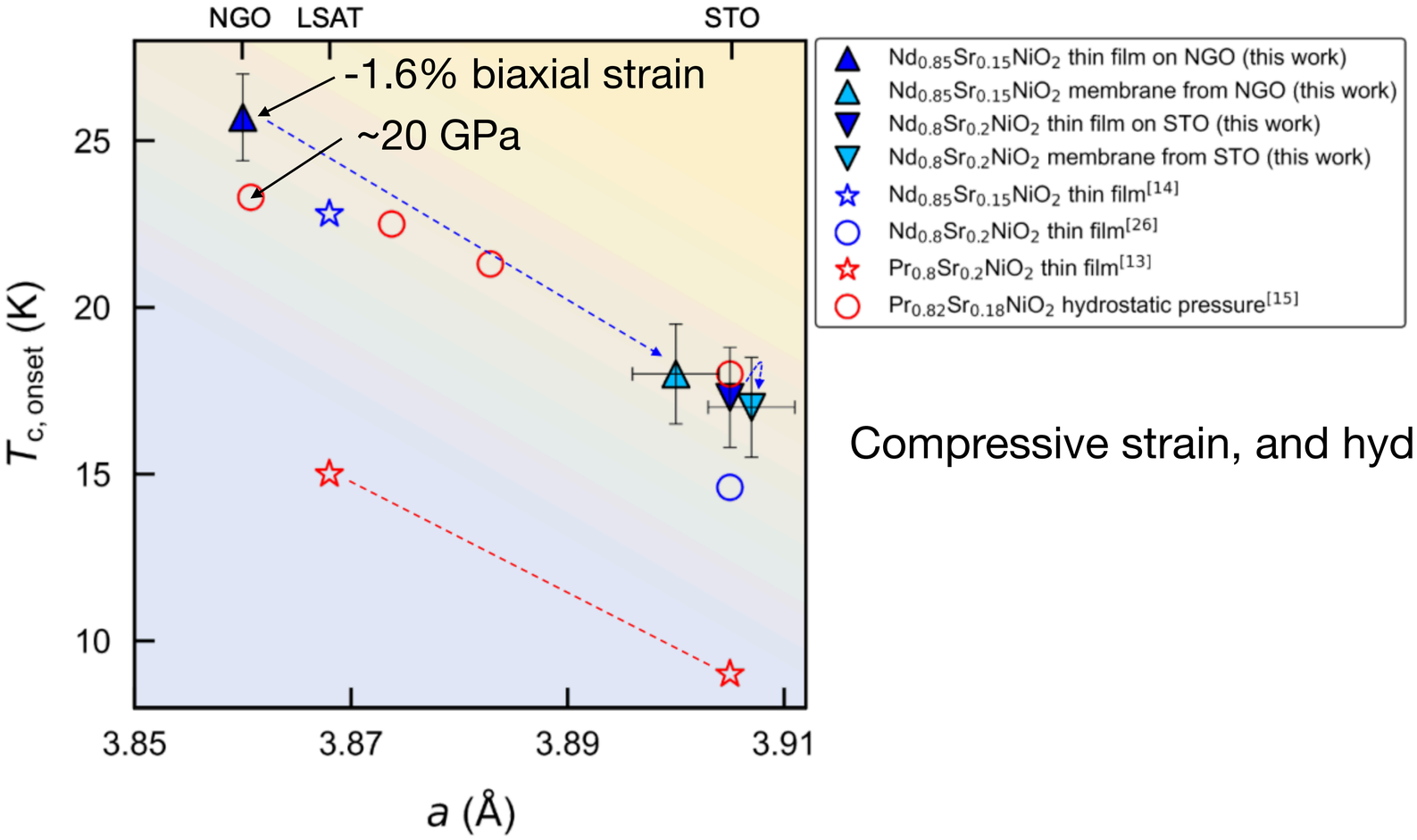






J. Fowlie et al, Nature Physics 18 (2022)

Maximizing critical temperature



Compressive strain, and hydrostatic pressure, increases T_c

Y. Lee et al, Nature Synthesis (2025)

Square-planar superconducting nickelates: Open questions

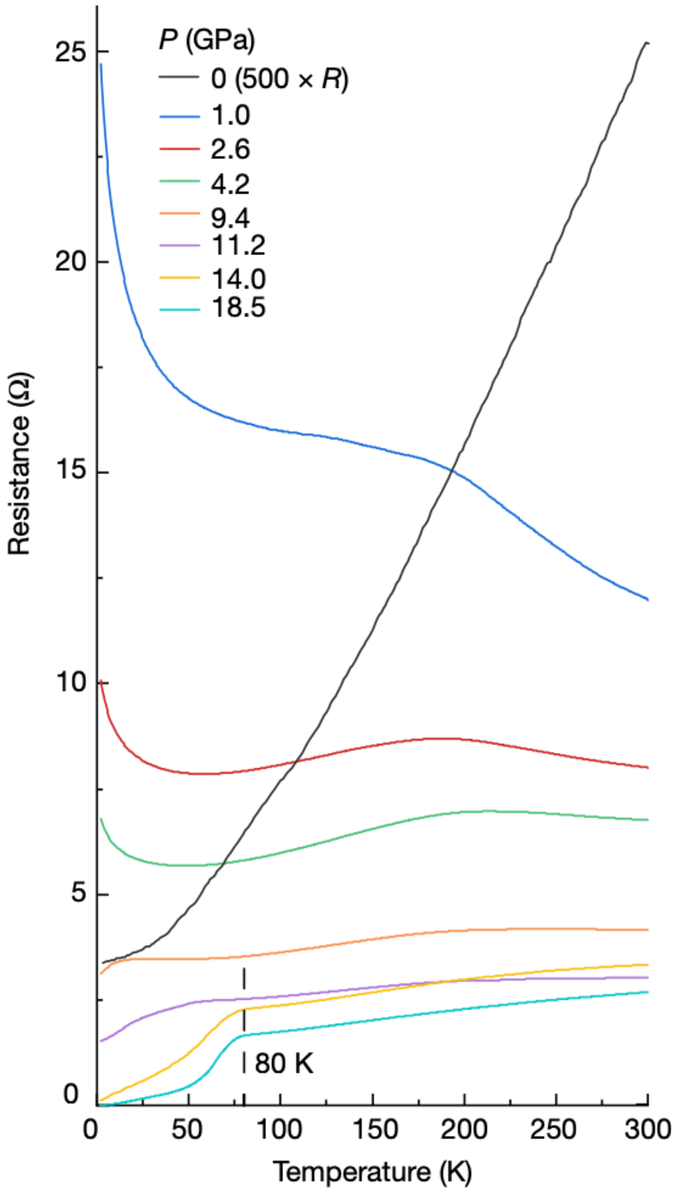
1. Why bulk samples are not superconducting?
2. Is there long-range magnetic order in the superconducting state?
3. What is maximum T_c?
4. Why are d^9 cuprates and d^9 nickelates so different?

Nickelates	**Cuprates**
Doped: Mott-Hubbard-like antiferromagnets	Doped: Charge-transfer-like, non-magnetic
Parent compound: Metallic, no long-range magnetic order Also superconduct	Parent compound: Insulating, long-range magnetic order

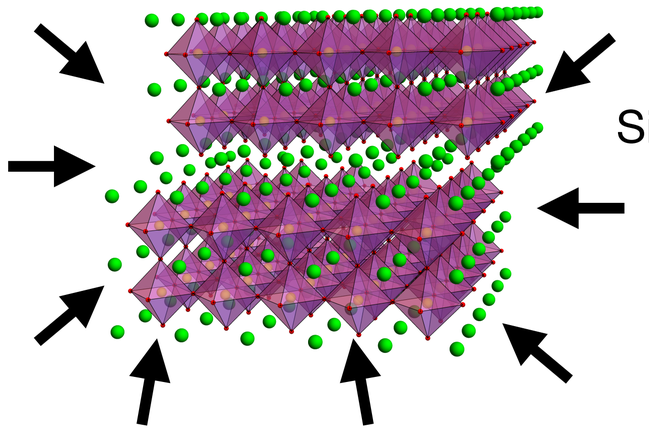
Cuprates recipe:

- Quasi-2-Dimensional ✓
- $3d^9$, Single hole in dx^2-y^2 orbital ✓
- Antiferromagnetic correlations ✗
- Strong TM *3d* - O *2p* hybridization ✗

Superconductivity in octahedral nickelates



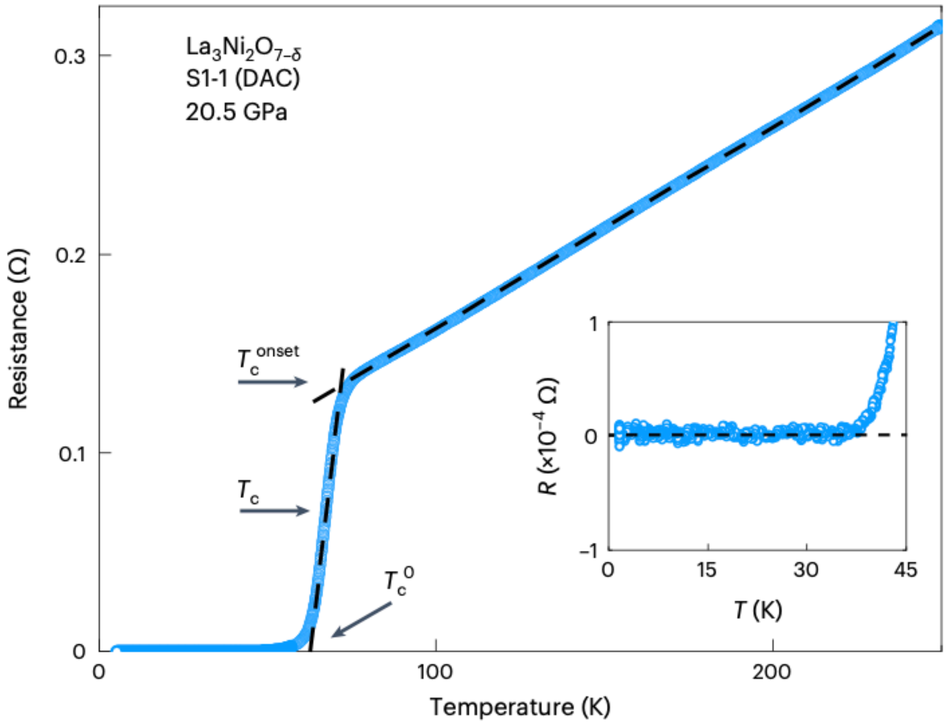
H. Sun et al, Nature 621(2023)



Single crystal $La_3Ni_2O_7$ at 20GPa

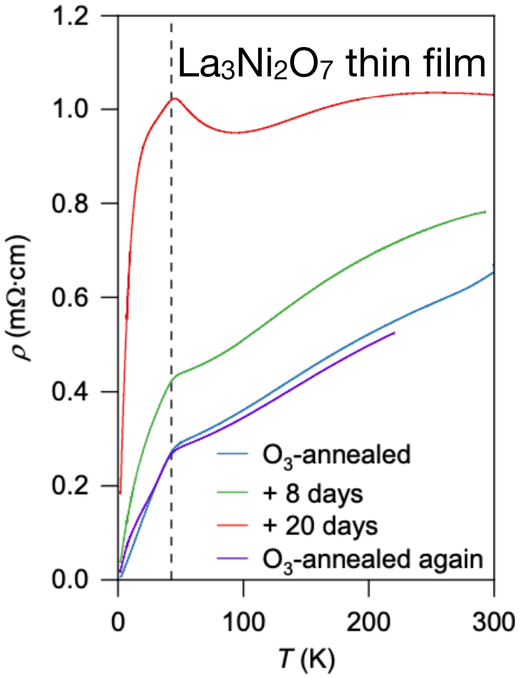
Extensively studied previously. Nobody looked at high pressure before?

$3d^{7.5}$ wasn't expected to be superconducting

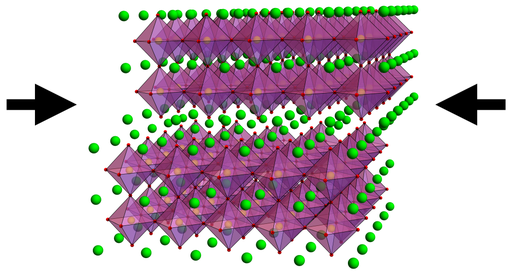


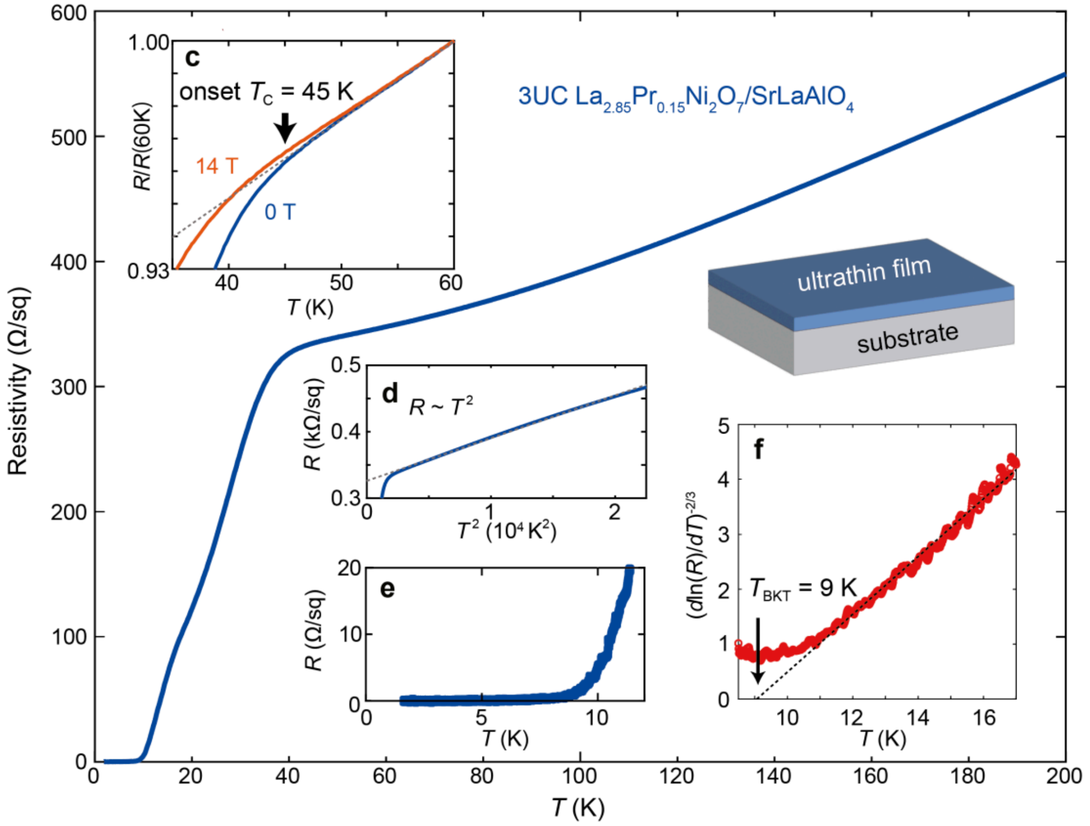
Y. Zhang et al, Nature Physics 20 (2024)

Superconductivity in octahedral nickelates at ambient pressure



E. K. Ko et al, Nature (2024)





G. Zhou et al, Nature (2025)

Extensively studied previously.
Nobody had good enough samples before, oxygen is crucial

Octahedral superconducting nickelates: Open questions

1. Is the superconductivity filamentary?
2. What is the physics…
    1. Similar to square-planar nickelates?
    2. Similar to cuprates?

Cuprates recipe:

- Quasi-2-Dimensional ✓
- $3d^9$, Single hole in dx^2-y^2 orbital ✗
- Antiferromagnetic correlations ?
- Strong TM *3d* - O *2p* hybridization ?