Superconductivity & electronic band structure in nickelates

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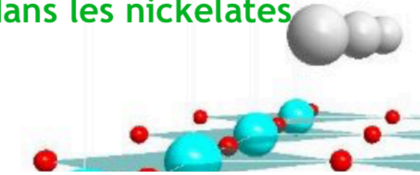


BIBLIOGRAPHIE SUPRACONDUCTIVITÉ NICKELATES

Article et commentaire publiés dans Nature le 27 aout 2019 :

Superconductivity in an infinite-layer nickelate D . Li, K. Lee, B. Yang Wang, M. Osada, S. Crossley, H. Ryoung Lee, Y Cui, Y. Hikita & H. Y. Hwang

Superconductivity seen in a nickel oxide G.A.Sawatzky

Articles publiés depuis le 27 aout 2019 :

28/08: Similarities and differences between infinite-layer nickelates and cuprates and implications for superconductivity A. S. Botana and M. R. Norman

30/08 : Model construction and a possibility of cuprate-like pairing in a new d^9 nickelate superconductor $(Nd,Sr)NiO_2$ H. Sakakibara, H. Usui, K. Suzuki, T. Kotani, H. Aoki ,and K. Kuroki

01/09: Hole superconductivity in infinite-layer nickelates J. E. Hirsch and F. Marsiglio

05/09 : Doped holes in $NdNiO_2$ and high-T_c cuprates show little similarity Mi Jiang, Mona Berciu, and George A. Sawatzky

05/09: Electronic structure of the parent compound of superconducting infinite-layer nickelates M. Hepting, D. Li, C. J. Jia, H. Lu, E. Paris, Y. Tseng, X. Feng, M. Osada, E. Been, Y. Hikita, Huang, D. J. Huang, Z. X. Shen, T. Schmit, H. Y. Hwang, B. Moritz, J. Zaanen, T. P. Devereaux, and W. S. Lee

06/09 : Robust $d_{x^2-y^2}$-wave superconductivity of infinite-layer nickelates X. Wu, D. Di Sante, T. Schwemmer, W. Hanke, H. Y. Hwang, S. Raghu, and R. Thomale

09/09 : Formation of 2D single-component correlated electron system and band engineering in the nickelate superconductor $NdNiO_2$ Y. Nomura, M. Hirayama, T. Tadano, Y. Yoshimoto, K. N

10/09 : Electronic structures and topological properties in nickelates $Ln_{n+1}Ni_nO_{2n+2}$ J. Gao, Z. Wang,C. Fang, and H. Weng

12/09 : Induced Magnetic Two-dimensionality by Hole Doping in Superconducting $Nd_{1-x}Sr_xNiO_2$ S. Ryee, H. Yoon, T. Jung Kim, M. Yong Jeong, and M. Joon Han

16/09 : Effective Hamiltonian for superconducting Ni oxides $Nd_{1-x}Sr_xNiO_2$ H. Zhang, L. Jin, S. Wang, B. Xi, X. Shi, F. Ye, and J.-W. Mei

17/09: A "road-map" of Nickelate superconductivity N. Singh

25/09: Self-doped Mott insulator for parent compounds of nickelate superconductors Guang-Ming Zhang, Yi-Feng Yang, Fu-Chun Zhang

27/09 : Kondo resonance and d-wave superconductivity in the t-J model with spin one holes: possible applications to the nickelate superconductor Nd1-xSrxNiO2Ya-Hui Zhang and Ashvin Vi

30/09 : Electronic structure of rare-earth infinite-layer ReNiO2 (Re=La, Nd) Peiheng Jiang, Liang Si, Zhaoliang Liao, Zhicheng Zhong

01/10 : Nickelate superconductors : Multiorbital nature and spin freezing Philipp Werner, Shintaro Hoshino

09/10 : Two-band model for magnetism and superconductivity in nickelates Lun-Hui Hu and Congjun Wu

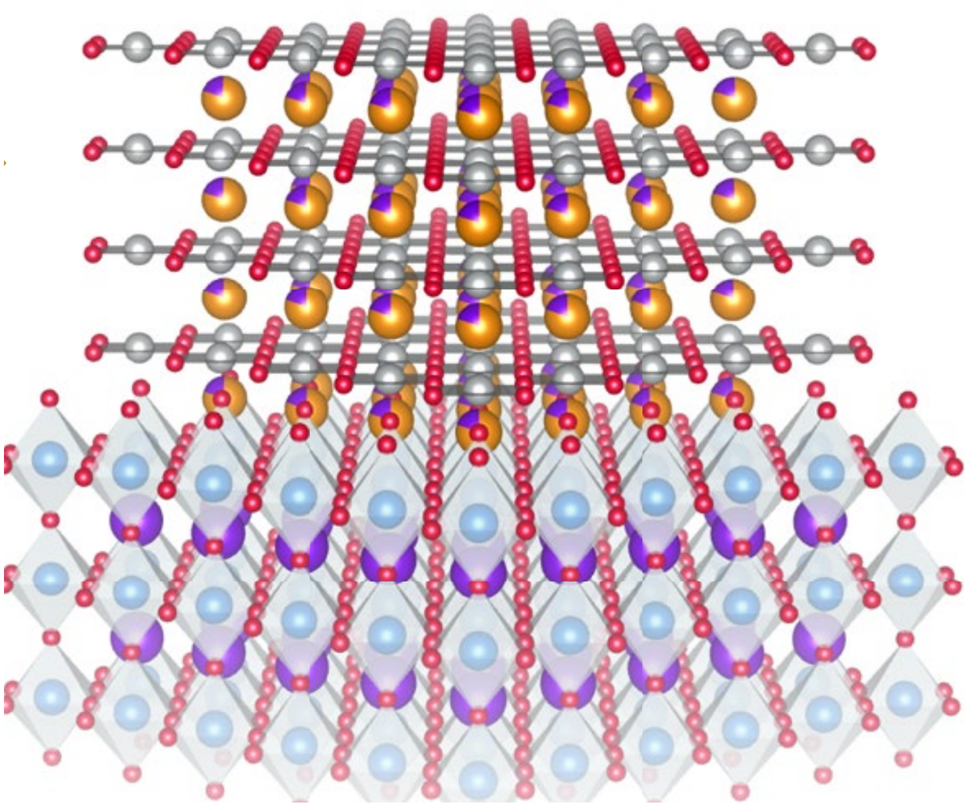
10/10 : Materials design of dynamically stable layered nickelates Motoaki Hirayama, Terumasa Tadano, Yusuke Nomura, Ryotaro Arita

15/10 : Spin excitations in nickelate superconductors Tao Zhou, Yi Gao, and Z. D. Wang

30/10 : Magnetic penetration depth and Tc in superconducting nickelates F. Bernardini, V. Olevano, A. Cano

Superconductivity

$Nd_{0.8}Sr_{0.2}NiO_2/SrTiO_3$ thin films (9 – 11 nm ≈ 30 unit cells)



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

Superconductivity

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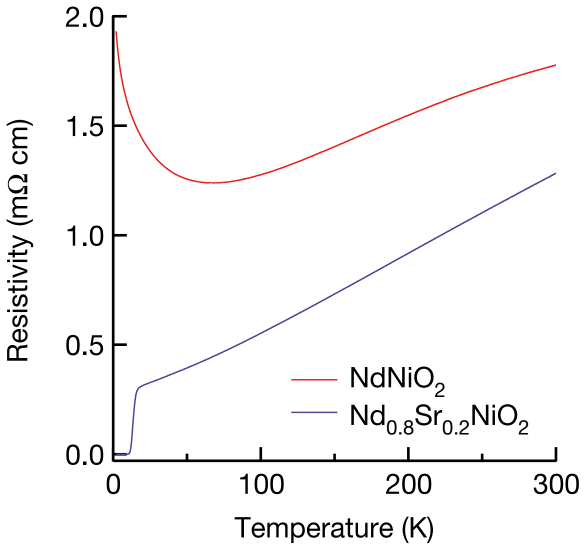
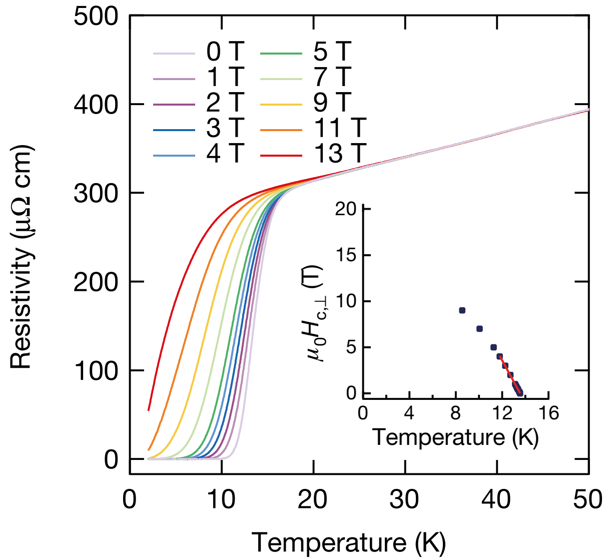
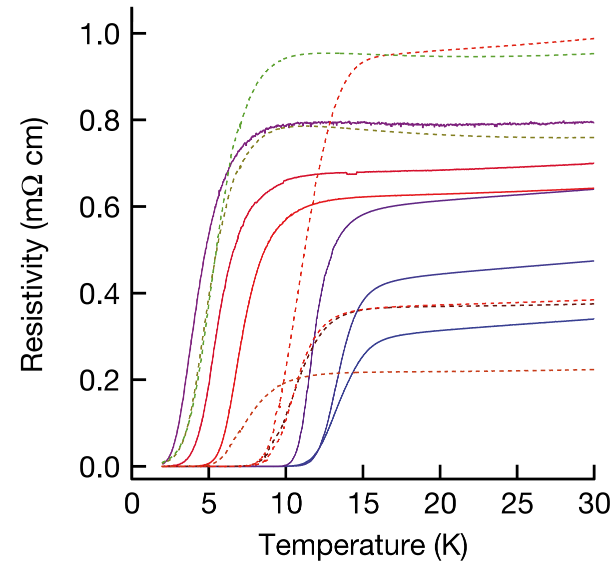




strongly sample dependent !



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

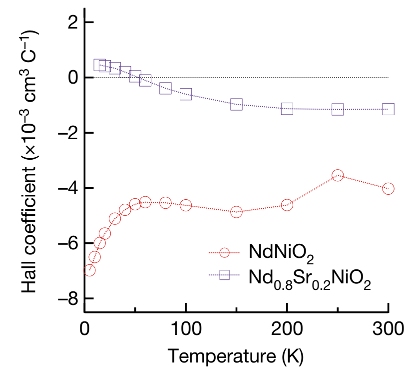
Superconductivity

Open questions

nickelates: paramagnetic metals vs. **cuprates**: AFM insulators

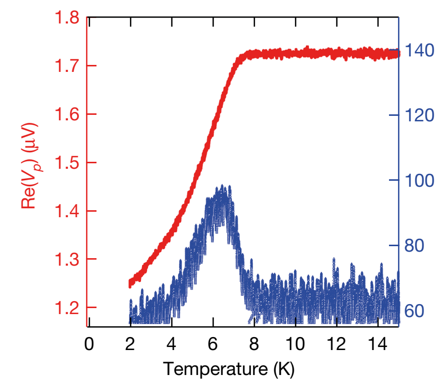
multiband?

The temperature-dependent normal-state Hall coefficient $R_H(T)$ is given in Fig. 3c. R_H for $NdNiO_2$ is negative at all temperatures, whereas it undergoes a sign change at about 55 K for $Nd_{0.8}Sr_{0.2}NiO_2$. This feature, as well as the overall magnitude of R_H, are inconsistent with the expectations for simple hole doping of a single electronic band, and suggest a more complex Fermi surface. This may be consistent with calculations of the electronic band structure of $LaNiO_2$, which find multiple electron and hole pockets that have different orbital contributions[6] and that vary with the Coulomb interaction.



type-II?

The fact that $\mathrm{Re}(V_p)$ does not approach zero at low temperatures resembles measurement results of a 40-nm-thick infinite-layer copper oxide film with $T_c \approx 10.8$ K and extrapolated London penetration depth $\lambda_L(T=0) = 2.2$ µm (ref. [31]). This indicates that λ_L for $Nd_{0.8}Sr_{0.2}NiO_2$ is similarly large compared to the film thickness. Given the numerical uncertainties arising from the finite sample size (substantially wider films show indications of laterally inhomogeneous reduction), the order parameter symmetry and the scale of disorder, we did not attempt to extract λ_L (ref. [32]). Nevertheless, these data suggest that this is a type-II superconductor



role of the interface?

We further note that the interface between the infinite-layer nickelate and the $SrTiO_3$ substrate (Fig. 1) hosts a strong polar discontinuity[30]. Depending on how this electrostatic boundary condition is resolved, there may be transport contributions from interface states. However, the comparison between $NdNiO_2$ and $Nd_{0.8}Sr_{0.2}NiO_2$ demonstrates that this alone does not lead to superconductivity here.

conventional
electron-phonon coupling SC?

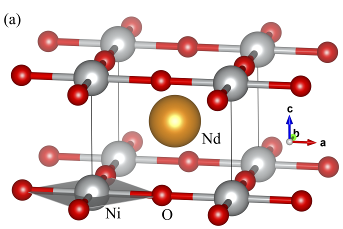
Li et al., Nature 572, 624 (2019)

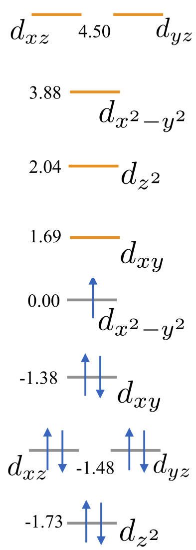
Electronic band structure

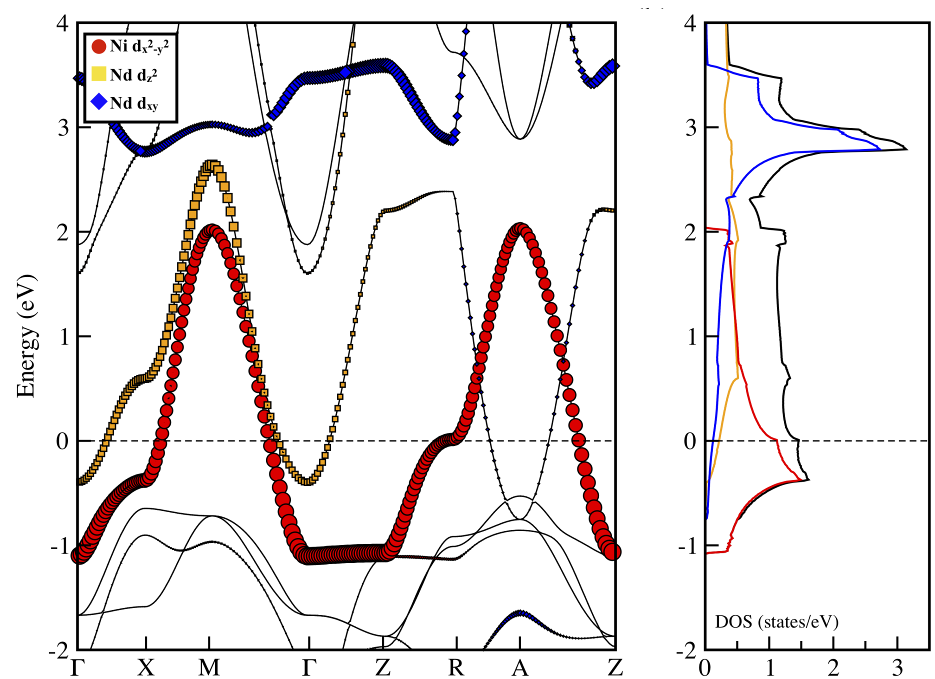
Electronic band structure

$R^{3+}Ni^{1+}(O^{-2})_2$ (R = La, Pr, Nd)

$3d^9$ configuration of Ni^{1+}, isoelectronic with Cu^{2+}







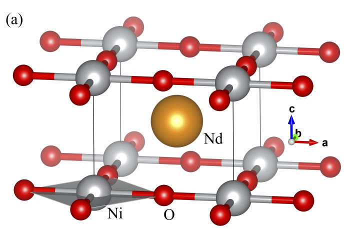
Lee & Pickett PRB 70, 165109 (2004)
Botana & Norman; arXiv:1908.10946
Shakakibara et al.; arXiv:1909.00060
Wu et al.; arXiv:1909.03015

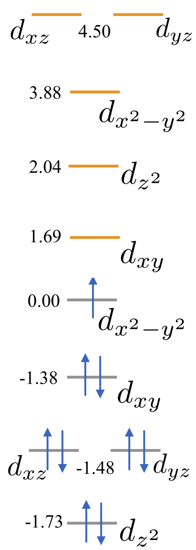
Bernardini, Olevano & Cano; arXiv:1910.13269

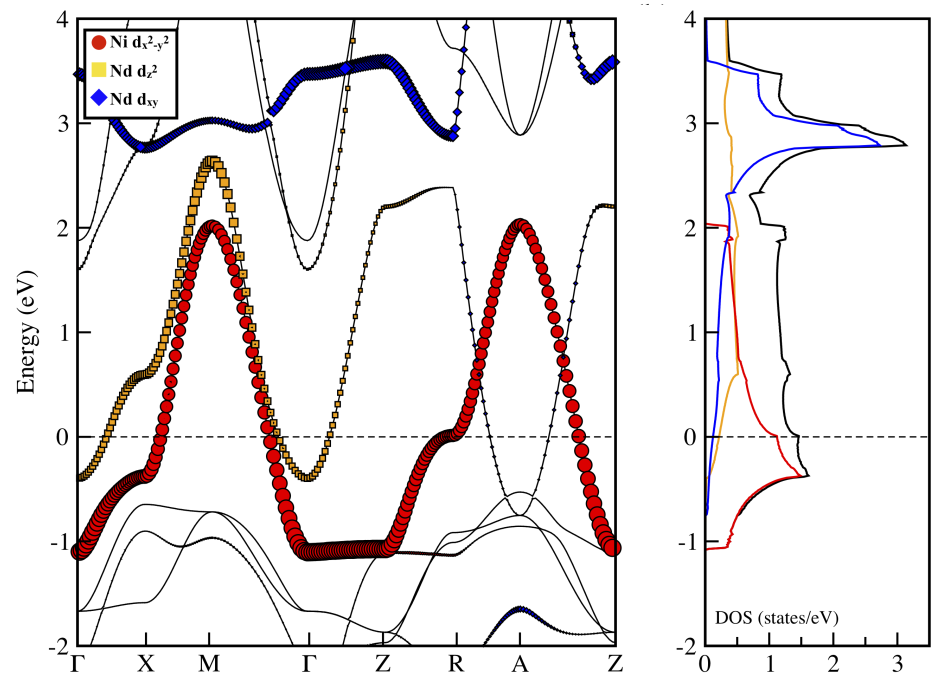
Electronic band structure

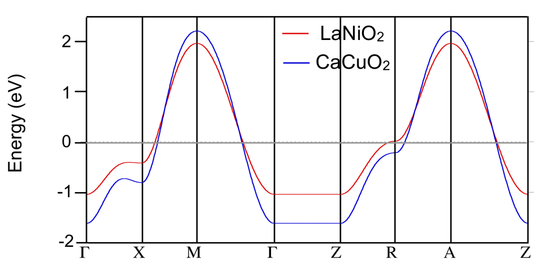
$R^{3+}Ni^{1+}(O^{-2})_2$ (R = La, Pr, Nd)

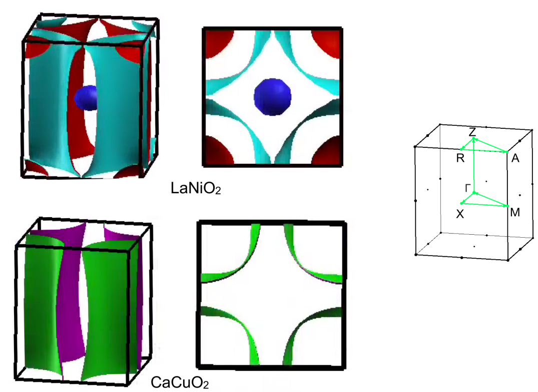
$3d^9$ configuration of Ni^{1+}, isoelectronic with Cu^{2+}







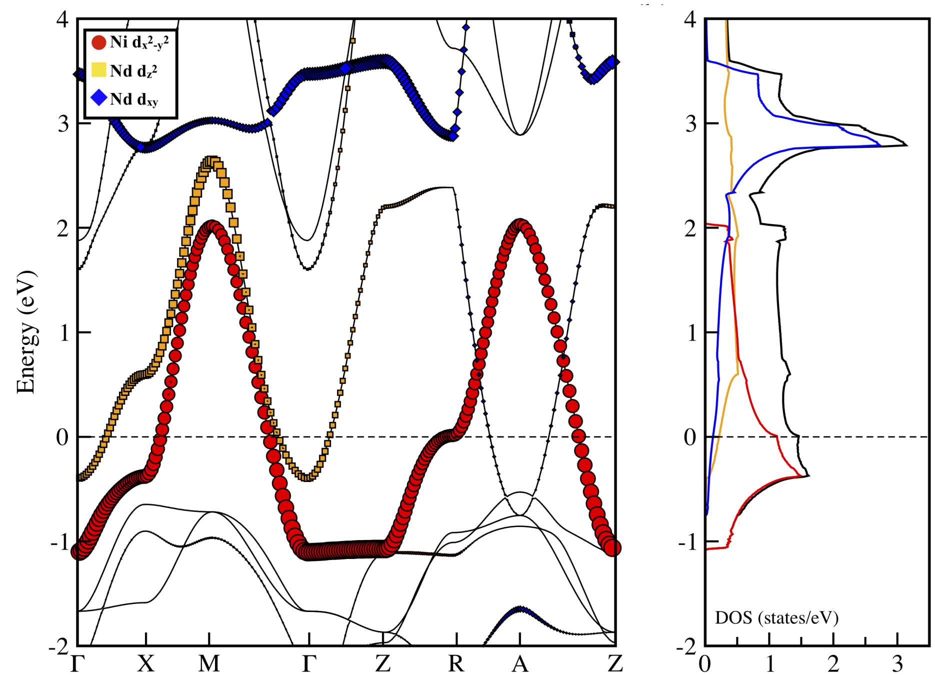


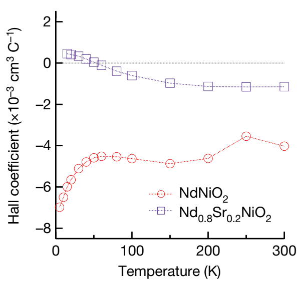


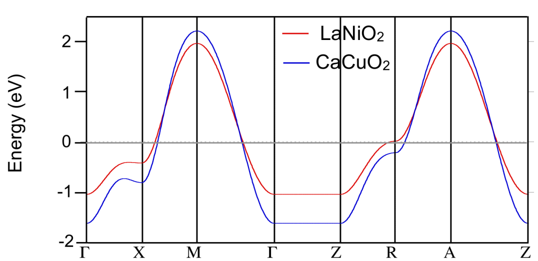
Electronic band structure

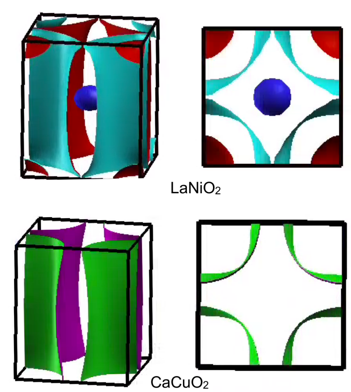
The La (Nd) $5d_{z^2}$ band crossing the Fermi level can naturally explain the metallic character of the *R*NiO$_2$ nickelates

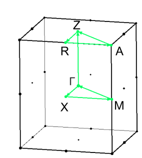
However, hole Fermi surface still needs to be somehow excluded to explain the Hall data. (???)











Electronic band structure

Electron-phonon coupling is **not enough** to mediate superconductivity

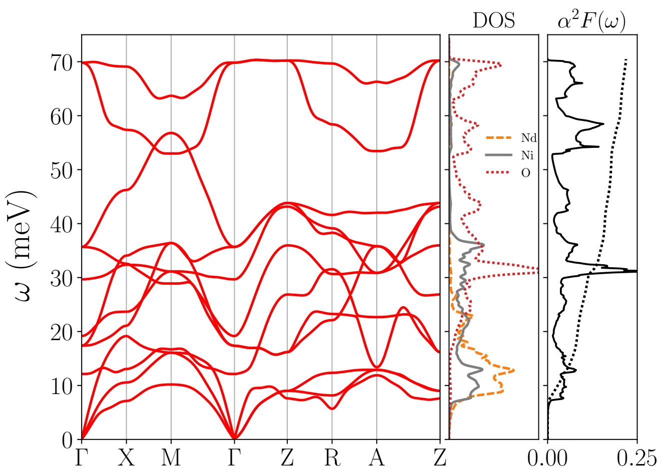


TABLE I. Electron-phonon interaction λ and the logarithmic average of phonon frequencies calculated for $NdNiO_2$ with different width of the Gaussian smearing. The T_c values are evaluated using the Allen-Dynes formula with $\mu^* = 0.1$.

Smearing width (Ry)	λ	ω_{ln} (K)	T_c (K)
0.04	0.22	283	0.00
0.06	0.28	258	0.06
0.08	0.32	249	0.24

Nomura et al.; arXiv:1909.03942v1

Electronic band structure

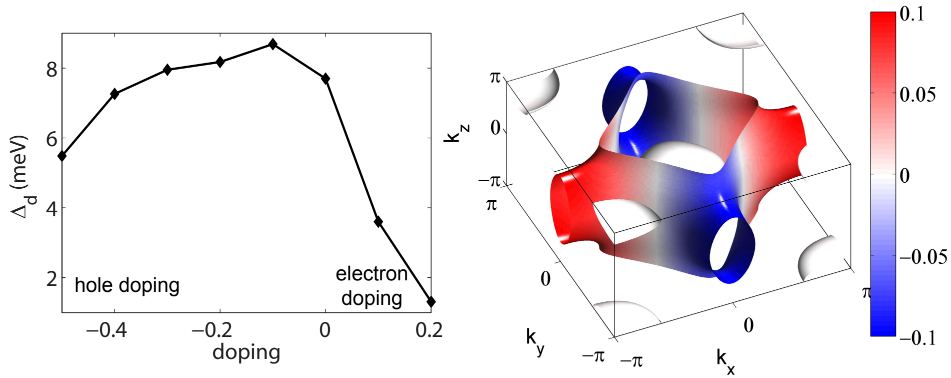
Spin fluctuations (weak coupling RPA approach) -> *d*-wave superconducting gap

Hubbard model

$$\begin{aligned} H_{\rm int} &= U_{\rm Ni}\sum_i n_{i3\uparrow}n_{i3\downarrow} + U_{\rm Nd}\sum_{i\mu} n_{i\mu\uparrow}n_{i\mu\downarrow} \\ &+ U'_{\rm Nd}\sum_{i,\mu<\nu} n_{i\mu}n_{i\nu} + J_{\rm Nd}\sum_{i,\mu<\nu,\sigma\sigma'} c^\dagger_{i\mu\sigma}c^\dagger_{i\nu\sigma'}c_{i\mu\sigma'}c_{i\nu\sigma} \\ &+ J'_{\rm Nd}\sum_{i,\mu\neq\nu} c^\dagger_{i\mu\uparrow}c^\dagger_{i\mu\downarrow}c_{i\nu\downarrow}c_{i\nu\uparrow} \end{aligned}$$

t-J **model**

$$H_J = \sum_{\langle ij\rangle} J_{ij}(\mathbf{S}_{i3}\mathbf{S}_{j3} - \frac{1}{4}n_{i3}n_{j3})$$

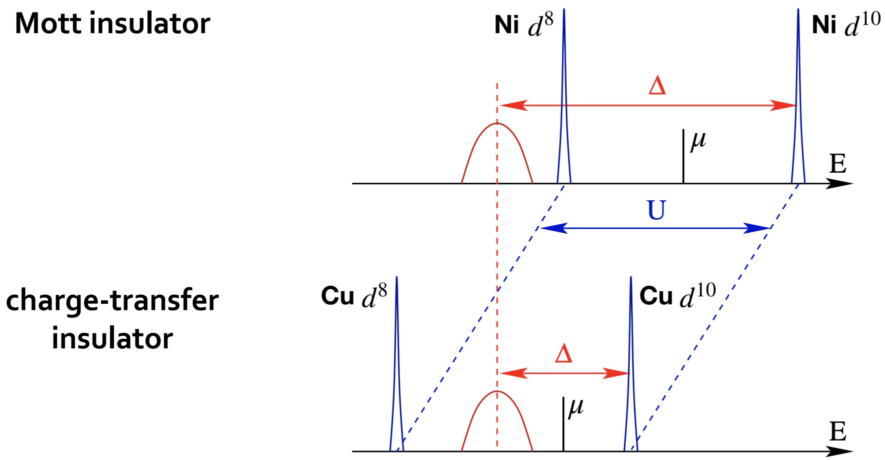


$d_{x^2-y^2}$-wave gap as a function doping

Wu et al.; arXiv:1909.03015
Shakakibara et al.; arXiv:1909.00060

Electronic band structure

Mott insulator vs charge-transfer insulator in the Zaanen-Sawatzky-Allen scheme



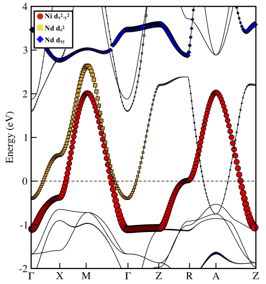
10 times smaller superexchange in the nickelates

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

no AFM & weakened spin fluctuations

Jiang, Berciu & Sawatzky; arXiv:1909.02557

Electronic band structure

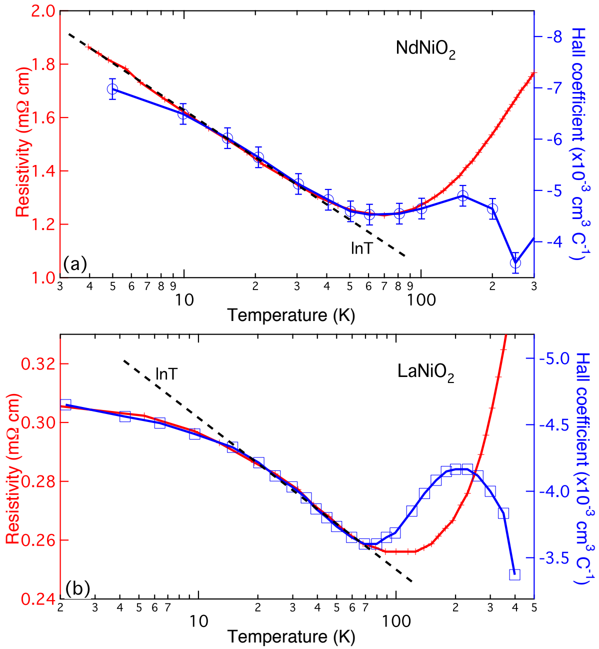


Nd and La $5d$ bands crossing the Fermi level
Kondo physics, beyond Kondo lattice (heavy fermions) and *t-J* model (cuprates)

RKKY -> exchange
holon - (S = 1) doublon excitations -> self-doped Mott state

Strange metals

$\rho \sim T^{\alpha}$ ($\alpha \simeq 1.12$)



Zhang et al.; arXiv:1909.11845
Zhang et al.; arXiv:1909.12865

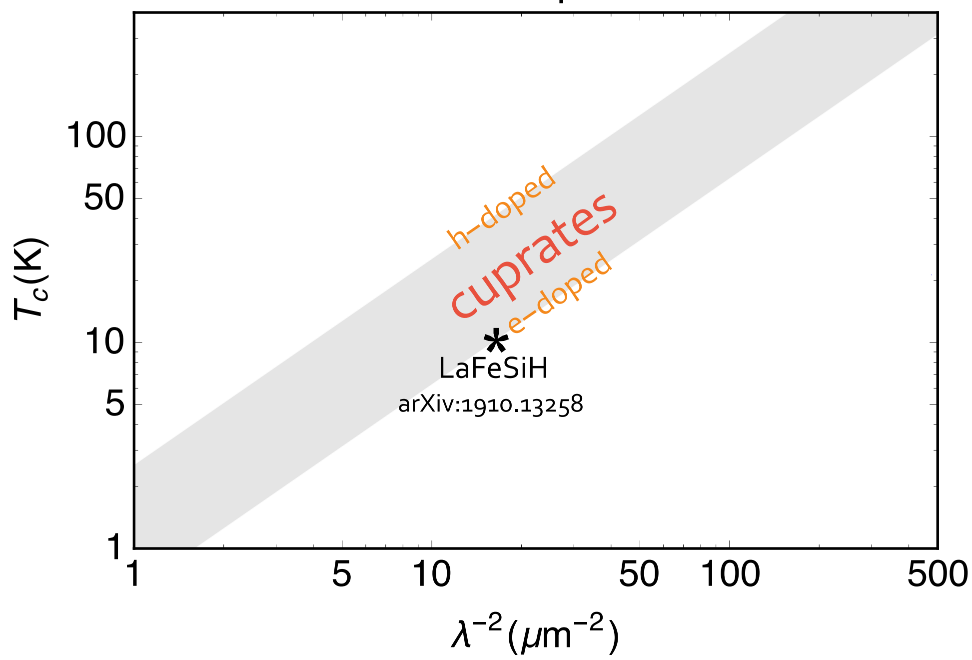
Electronic band structure

London penetration depth

$$(\lambda^2)^{-1}_{ij} = \underbrace{\frac{\mu_0 e^2}{4\pi^3\hbar} \oint_{\rm FS} dS \left[\frac{v_{Fi}v_{Fj}}{v_F}\right.}_{\lambda(T=0)} \left(1 + 2\int_\Delta^\infty \left(\frac{\partial f}{\partial E}\right) \frac{E dE}{\sqrt{E^2-\Delta^2}}\right)\Bigg]$$

$\lambda(T=0)$ is just a band-structure property!

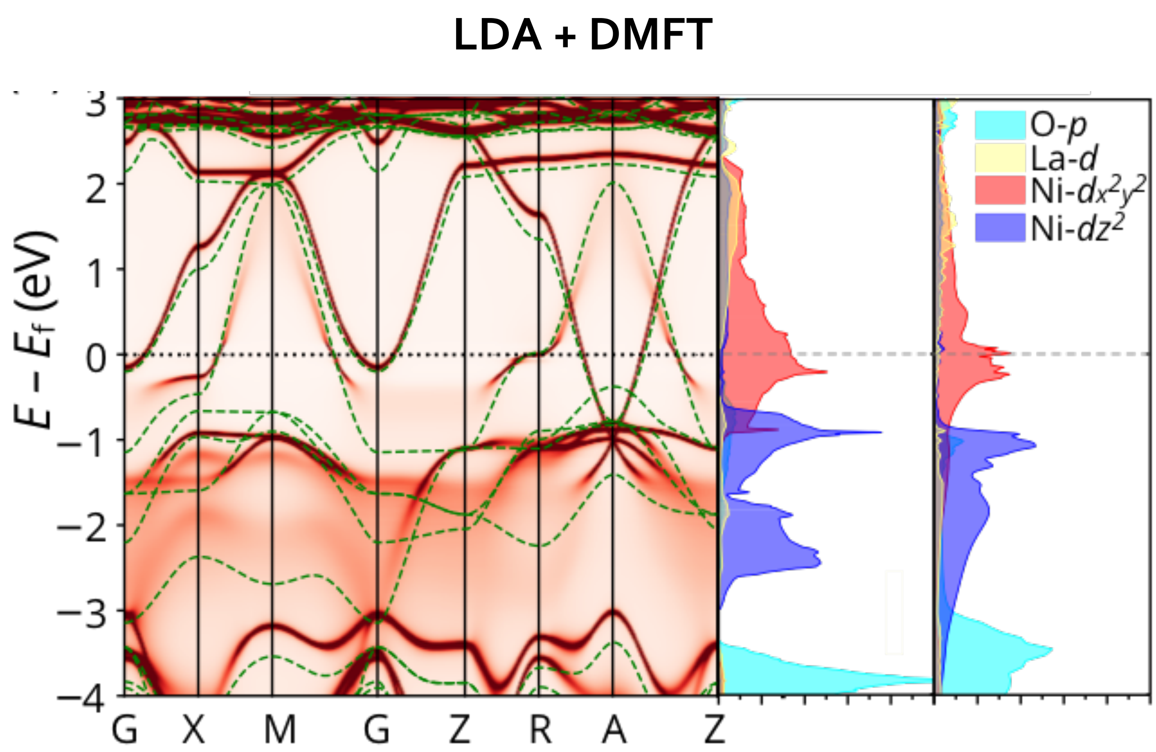
Uemura plot



Nickelates: i) are potential room-temperature superconductors,
ii) or have nothing to do with cuprates,
iii) or their electronic band structure needs to be seriously revisited

Bernardini, Olevano & Cano; arXiv:1910.13269

Electronic band structure



Ryee et al.; arXiv: 1909.05824