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SUPPLEMENTARY INFORMATION

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Electronic structure of the parent compound of superconducting infinite-layer nickelates

M. Hepting[1,8], D. Li[1], C. J. Jia[1*], H. Lu[1], E. Paris[2], Y. Tseng[2], X. Feng[1], M. Osada[1], E. Been[1], Y. Hikita[1], Y.-D. Chuang[3], Z. Hussain[3], K. J. Zhou[4], A. Nag[4], M. Garcia-Fernandez[4], M. Rossi[1], H. Y. Huang[5], D. J. Huang[5], Z. X. Shen[1,6], T. Schmitt[2], H. Y. Hwang[1], B. Moritz[1], J. Zaanen[7], T. P. Devereaux[1] and W. S. Lee[1*]

[1]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [2]Photon Science Division, Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland. [3]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [4]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK. [5]NSRRC, Hsinchu Science Park, Hsinchu, Taiwan. [6]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford, CA, USA. [7]Instituut-Lorentz for theoretical Physics, Leiden University, Leiden, the Netherlands. [8]Present address: Max Planck Institute for Solid State Research, Stuttgart, Germany.
*e-mail: chunjing@stanford.edu; leews@stanford.edu

Supplementary Information
for
Electronic structure in the parent compound of superconducting infinite-layer nickelates

M. Hepting[1†], D. Li[1], C. J. Jia[1*], H. Lu[1], E. Paris[2], Y. Tseng[2], X. Feng[1], M. Osada[1], E. Been[1], Y. Hikita[1], Y.-D. Chuang[3], Z. Hussain[3], K. J. Zhou[4], A. Nag[4], M. Garcia-Fernandez[4], M. Rossi[1], H. Y. Huang[5], D. J. Huang[5], Z. X. Shen[1,6], T. Schmitt[2], H. Y. Hwang[1], B. Moritz[1], J. Zaanen[7], T. P. Devereaux[1], and W. S. Lee[1*]

[1]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory and Stanford, Menlo Park, California 94025, USA

[2]Photon Science Division, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

[3]Advanced Light Source, Lawrence Berkeley National Laboratory

[4]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom

[5]NSRRC, Hsinchu Science Park, Hsinchu 30076, Taiwan

[6]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford, CA 94305, USA.

[7] Instituut-Lorentz for theoretical Physics, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands.

Correspondence to: chunjing@stanford.edu and leews@stanford.edu

Present address:

†Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

This Supplementary Information Contains:

Supplementary Table 1-3

Unit eV		Ni [0,0,0]					O[0, ½, 0]			O[½, 0, 0]			La [½,½,½]
		d_{z2}	d_{x2-y2}	d_{xy}	d_{xz}	d_{yz}	p_z	p_x	p_y	p_z	p_x	p_y	d_{z2}
Ni [0,0,0]	d_{z2}	-0.04							-0.3		0.3		-0.5
	d_{x2-y2}		0.70						-1.2		-1.2		
	d_{xy}			-0.1				0.7				0.7	
	d_{xz}				0					-0.8			-0.1
	d_{yz}					0	0.8						0.1
O [0, ½, 0]	p_z					0.8	-2.32	0.2					0.4
	p_x			0.7			0.2	-2.34			0.3	0.2	-0.2
	p_y	-0.3	-1.2						-3.26		0.6	0.3	0.4
O [½, 0, 0]	p_z				-0.8					-2.32		-0.2	0.4
	p_x	0.3	-1.2					0.3	0.6		-3.25		-0.4
	p_y			0.7				0.2	0.3	-0.2		-2.35	0.2
La [½,½,½]	d_{z2}	-0.5			-0.1	0.1	0.4	-0.2	0.4	0.4	-0.4	0.2	2.42

Supplementary Table 1: Material parameters for $LaNiO_2$ obtained from Wannier downfolding. The diagonal terms represent on-site energies. The off-diagonal terms represent the hopping between two orbitals. The shaded area only shows those parameters whose absolute value is larger than 0.1. All values are in units of eV. The triplet [i,j,k] appearing next to each orbital shows its

relative position within a one Ni, $LaNiO_2$ tetragonal unit cell along the unit a, b, and c axes, respectively, with Ni at [0,0,0].

Orbital configuration		Approximate percentage	Dipole transition spin up (minority spin)	Dipole transition spin down (majority spin)
d^9	$d^4 \uparrow d^5 \downarrow$	56%	Yes	No
d^8R	$d^3R \uparrow d^5 \downarrow$	24%	Yes	No
	$d^4 \uparrow d^4R \downarrow$	14%	Yes	Yes
d^7R^2	$d^3R \uparrow d^4R \downarrow$	6%	Yes	Yes

Supplementary Table 2: Orbital configurations and their approximate percentage shown in the many-body ground state calculation. Here, R represents a rare earth electron in the La cage surrounding each Ni, in analogy to the standard ligand hole ($\underline{L}$), due to hybridization between Ni and La. This is akin to charge transfer, but from Ni to the rare earth, instead of oxygen to transition metal more commonly encountered in oxides.

Hopping Parameters from Wannier Downfolding			
i	j	k	$t^{R}_{[i,j,k]}$
0	0	0	1.132
0	0	1	-0.022
0	0	2	-0.112
0	0	3	0.019
1	0	0	-0.028
1	0	1	-0.164
1	0	2	0.033
1	1	0	-0.062
1	1	1	0.024
1	1	2	0.013
1	1	3	-0.019
2	0	1	0.009
2	1	1	0.009
i	j	k	$t^{Ni}_{[i,j,k]}$
0	0	0	0.267
1	0	0	-0.355
1	1	0	0.090
2	0	0	-0.043
0	0	1	-0.043
1	1	1	0.013
i	j	k	$t^{R-Ni}_{[i,j,k]}$
2	0	0	-0.026
2	0	2	0.013

Supplementary Table 3: Tight-binding model parameters for the two-orbital model for $LaNiO_2$. The elements in the table show all independent hopping parameters with an absolute magnitude larger than 0.008 eV. The triplet of integers [i,j,k] represents hopping between unit cells with a relative separation r = i a + j b + k c, where a, b, and c are unit vectors in the respective directions. Here, for simplicity we take a=b=c=1 and measure all momenta kx, ky, and kz, accordingly. Tetragonal symmetry dictates that for the rare earth- (*R*-) and Ni-band parameters, the hopping with triplet [i,j,k] would be equivalent to [-i,j,k], [i,-j,k], [i,j,-k], [-i,-j,k], [-i,j,-k], [i,-j,-k], [-i,-j,-k], and all combinations with i ↔ j, with a phase factor of 1 or -1 depending on the symmetry of the orbitals. The triplet [0,0,0] represents the orbital site energy ε_0. The La-centered and Ni-centered Wannier orbitals have relative unit cell coordinates [0.5, 0.5, 0.5] and [0.0, 0.0, 0.0], respectively,

which only affects the equivalent triplets for the cross-orbital-hybridization terms $t^{R\text{-}Ni}$. The Fermi energy E_F is at 0 eV.