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Phys. Rev. B **101**, 020503 — Published 10 January 2020

DOI: 10.1103/PhysRevB.101.020503

Role of $4f$ states in infinite-layer $NdNiO_2$

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(Dated: December 18, 2019)

Atomic $4f$ states have been found to be essential players in the physical behavior of lanthanide compounds, at the Fermi level E_F as in the proposed topological Kondo insulator SmB_6, or further away as in the magnetic superconductor system $\mathcal{R}Ni_2B_2C$ ($\mathcal{R}$=rare earth ion) and in $Y_{1-x}Pr_xBa_2Cu_3O_7$, where the $4f$ shell of Pr has a devastating effect on superconductivity. In hole-doped $\mathcal{R}NiO_2$, the $\mathcal{R}$=Nd member is found to be superconducting while $\mathcal{R}$=La is not, in spite of the calculated electronic structures being nearly identical. We report first principles results that indicate that the Nd $4f$ moment affects states at E_F in infinite-layer $NdNiO_2$, an effect that will not occur for $LaNiO_2$. Treating 20% hole-doping in the virtual crystal approach indicates that 0.15 holes empty the Γ-centered Nd-derived electron pocket while leaving the other electron pocket unchanged; hence Ni only absorbs 0.05 holes; the La counterpart would behave similarly. However, coupling of $4f$ states to the electron pockets at E_F arises through the Nd intra-atomic $4f-5d$ exchange coupling $K \approx 0.5$ eV and is ferromagnetic (FM), *i.e.* anti-Kondo, in sign. This interaction causes spin-disorder broadening of the electron pockets and should be included in models of the normal and superconducting states of $Nd_{0.8}Sr_{0.2}NiO_2$. The Ni moments differ by $0.2\mu_B$ for FM and antiferromagnetic alignment (the latter are larger), reflecting some itineracy and indicating that Heisenberg coupling of the moments may not provide a quantitative modeling of Ni-Ni exchange coupling.

I. BACKGROUND AND MAJOR ISSUES

The discovery of superconductivity up to T_c=15 K in Sr-doped $NdNiO_2$ ($Nd_{0.8}Sr_{0.2}NiO_2$)[1] has re-invigorated the three decade long issue of whether there may be nickelates that can host cuprate-type superconductivity. $LaNiO_2$, which is isostructural with "infinite layer" $CaCuO_2$[2] that superconducts up to 110 K when doped,[3] has been one of the prime candidates, but what doping is possible has never resulted in superconductivity. $NdNiO_2$ is also isovalent with $CaCuO_2$, providing a nominal d^9 configuration on the open shell transition metal ion.

Early comparison of the electronic structures of $CaCuO_2$ and $NdNiO_2$ identified similarities but substantial differences,[4, 5] with questions about whether concepts such as strong superexchange coupling of the transition metal moments, or of Zhang-Rice singlets upon doping,[1] are relevant to this nickelate. A number of groups recently have revisited this question, with the objective of few-band model-building to quantify differences related to superconductivity.[6–19] The popular approach has been to obtain the non-magnetic local density approximation (LDA) band structure of $NdNiO_2$ with the $4f^3$ electrons assigned to a non-magnetic core, then approximate the low energy bands with a minimal local orbital model, add a repulsive local interaction, and evaluate the consequences, *viz.* the pairing susceptibility. Close attention is given to the geometry of the Fermi surface (FS), which strongly impacts the pairing susceptibility.

Detailed analyses of the LDA electronic structure have been provided by Botana and Norman[6] for $LaNiO_2$ and by Nomura *et al.*[9] for $NdNiO_2$, in which three nonmagnetic $4f$ electrons are included in the Nd core. In addition to the roughly half-filled Ni $3d_{x^2-y^2}$ band, several groups find and quantify Nd $5d$ derived bands obtained earlier.[4, 5] A Nd $5d_{z^2}$ band drops below the Fermi level E_F at Γ, and in addition a band usually identified as Nd $5d_{xy}$-derived drops below E_F at the zone corner A=(π,π,π) point [in units of $(\frac{1}{a},\frac{1}{a},\frac{1}{c})$]. This undoped $NdNiO_2$ FS differs in significant ways from that of nonmagnetic $CaCuO_2$ but is similar to $LaNiO_2$. X-ray absorption spectra of the O K and Ni L_3 edges[20] do not reveal significant differences between $LaNiO_2$ and $NdNiO_2$.

There are other fundamental questions to be considered. Experimentally, undoped $CaCuO_2$ orders antiferromagnetically with a high Neel temperature of 442 K,[21] while undoped $NdNiO_2$ and $LaNiO_2$ do not order.[1] The underlying differences with cuprates are several. The mean Ni $3d$ level ϵ_d is separated from the O $2p$ level ϵ_p by 4 eV in the nickelates versus only 2 eV in the cuprate.[6] Ni therefore has less hybridization with oxygen $2p$ orbitals than does Cu, thus should have a stronger tendency toward local moment magnetism than does Cu, and indeed it does so in LDA calculations. The superexchange coupling J is much smaller for the nickelate,[6] thus one expects a lower but nonzero Neel temperature.

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Finally, $LaNiO_2$ and $NdNiO_2$ are reported as conducting (albeit poorly), whereas $CaCuO_2$ is insulating. Lack of Ni ordering is a central question to address; however, both in calculations and experimentally the nickelates are conducting. We note that magnetic order disappears in cuprates when they are doped to become conducting.

The model treatments mentioned above would suggest that doped $LaNiO_2$ should be superconducting as is doped $NdNiO_2$. Since this is not the case, we pursue the viewpoint that a more fundamental question is what features may account for this difference between two highly similar nickelates. La and Nd are very similar chemically, with tri-positive ionic radii only slightly larger for La than for Nd. Although small size differences in lattice constants or strains can influence states in correlated insulators, itineracy and screening by carriers strongly reduce such effects.

An obvious difference between these nickelates is that La^{3+} is closed shell and nonmagnetic whereas Nd^{3+}, with Hund's rule ground state $S = \frac{3}{2}, L = 6, J = \frac{9}{2}$, has a (free ion) Curie-Weiss moment of nearly 4 μ_B. Superconductivity appears in $Nd_{0.8}Sr_{0.2}NiO_2$ in the midst of these large disordered local moments, which should compete with superconducting phases, directly or by introducing disorder into the electronic structure. In several YBCO-type cuprates, however, replacing a nonmagnetic rare earth ion (La or Y) by a magnetic lanthanide from Dy to Tb does not affect the superconductivity, because the small $4f$ orbital is not involved in the electronic structure. Surprisingly, $PrBa_2Cu_3O_7$ was found to be non-superconducting,[22] due to antibonding coupling of the Pr $4f_{z(x^2-y^2)}$ orbital to the O $2p$ orbitals.[23, 24] Notably, the local environment of the $4f$ ion is the same as in $NdNiO_2$.

Another related system is the rare earth nickel borocarbides $\mathcal{R}Ni_2B_2C$ where $\mathcal{R}$ can be one of many of the rare earth atoms. This system displays strong interplay and competition between the $\mathcal{R}$ $4f$ magnetic moment and the conduction states with heavy Ni character, with the $\mathcal{R}$ $5d$ playing an important role in coupling the local moments to the itinerant states.[25, 26] Elemental europium at high pressure but retaining a f^7 local moment, switches from metallic and magnetically ordered to superconducting and magnetically disordered around 80 GPa,[27, 28] providing its own questions about the effect of $4f$ moments on pairing, a coupling that must proceed through the Eu $5d$ states.

The question of possible impact of the $4f$ shell has not been addressed in $NdNiO_2$. While direct $4f$-nickelate hybridization may be small, there is an intra-atomic exchange coupling between the $4f$ spin and the $5d$ states around E_F that, as mentioned, does not occur in $LaNiO_2$. Since the $5d$ bands cross E_F, carriers will be affected. Specifically, with disordered Nd moments, the $5d$ on-site energies will be spin-split, with a projection along any given direction that is distributed randomly. A carrier in a $5d$ band will be subjected to a random potential, resulting in band broadening and magnetic scattering that is absent in $LaNiO_2$.

The presentation is organized as follows. The computational methods and material configurations are described in Sec. II. In Sec. III results are presented for four assumed types of magnetic order in $NdNiO_2$. The electronic bands and Fermi surfaces for non-magnetic Ni are discussed in Sec. IV. A few results relating to the occupied Nd $4f$ orbitals are presented in Sec. V, followed by discussion of hole doping in Sec. VI. Some observations about the effects of magnetic order and relation to other $4f$-containing superconductors are made in Sec. VII, which is followed by a brief summary in Sec. VIII.

II. COMPUTATIONAL METHODS

We have studied the electronic and magnetic properties of $NdNiO_2$ using the precise, all-electron, full potential linearized augmented planewave method as implemented in WIEN2K[29]. The lattice constants $a = 3.92$ Å, $c = 3.37$ Å observed for superconducting $Nd_{0.8}Sr_{0.2}NiO_2$[1] have been used, all atoms lie at $P4/mmm$ symmetry determined positions. Strong intra-atomic interactions on Nd, and usually on Ni in nickelates, are modeled with the DFT+U method[30] (density functional theory plus Hubbard U), which is essential to preserve the $4f$ local moment and place the corresponding bands away from E_F. The fully anisotropic, rotationally invariant DFT+U correlation correction functional in the fully localized limit form[31] implemented in WIEN2K, was used. Results are presented for U_f^{Nd}=8.0 eV, J_f^{Nd}=1.0 eV, U_d^{Ni}=5.0 eV, J_d^{Ni}=0.7 eV (and occasionally for U_d^{Ni}=0). Other input parameters and a survey of results beyond those presented here are provided in the Supplemental Material (SM).[32] Sec. VI were carried out by reducing the nuclear charge on Nd by 0.20, and removing the same amount of electrons.

The strong local $4f$ moment requires magnetically ordered calculations. We find that Ni prefers a moment of the order of 0.5 μ_B without any U^{Ni}, which increases to $\sim$1 μ_B for the values we have used. The Nd moment always assumes the spin value of 3 μ_B characteristic of an f^3 Hund's rule ion, plus minor exchange polarization of the $5d$ orbitals. We have studied four magnetic configurations:
AFM0: AFM Nd layers with non-magnetic Ni layers;
AFM1: both Ni and Nd layers have antialigned moments;
AFM2: FM Nd layers and AFM Ni layers;
FM: all Nd and Ni moments aligned.
Note that it is the AFM1 and AFM2 cases in which Ni is antiferromagnetically ordered. Note also that AFM0 is done with U_d^{Ni}=0, so its energy cannot be compared with the other cases.

The SM provides additional information about the electronic structures. An insulating band structure is never obtained, which is a great difference compared with cuprates. It was shown earlier that increasing U on Ni in $NdNiO_2$ never leads to a Mott insulator, instead a $3d_{z^2}$

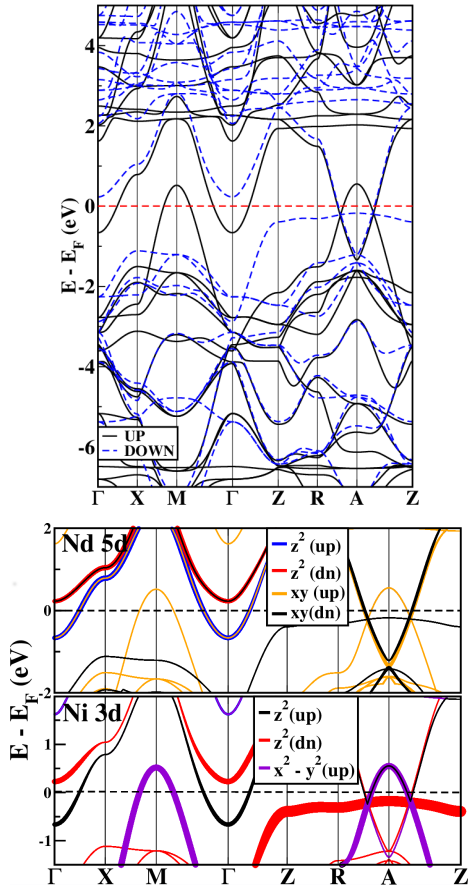

FIG. 1: Top: GGA+U FM bands of $NdNiO_2$: solid lines denote majority, dashed lines indicate minority, and E_F is the zero of energy. Bottom: Color fatband plot of FM $NdNiO_2$ near E_F, with the legend describing the color choice. Note the Nd-derived electron pockets at Γ and A, and the Ni majority $d_{x^2-y^2}$ hole pockets at M and A.

orbital becomes unoccupied and forms a peculiar intra-atomic singlet with the $d_{x^2-y^2}$ orbital.[5]

III. MAGNETIC ORDER

Although it is expected that Ni^{1+} d^9 ions will tend to order in antiferromagnetic (AFM1 or AFM2) fashion through superexchange as does $CaCuO_2$ and several other d^9 cuprates, we begin with FM alignment within both Ni and Nd layers, as it enables identification of the intra-atomic exchange splitting between the occupied Nd $4f$ and conduction $5d_{z^2}$ orbitals.

A magnetic Ni ion leads to a 120 meV energy gain compared to non-magnetic. This exaggerated tendency toward magnetic ordering and the magnitude of the magnetic moment are a known deficiency of (semi)local density functional methods, with much of the problem attributed to the lack of effects of spin fluctuations in the functional.

The energies can be compared for those cases with magnetic Ni (AFM1, AFM2, FM) for which the same functional is used. The energy of AFM2 (FM Nd) is slightly lower than that of AFM1 (AFM Nd), by 7 meV for U^{Ni}=0 and by only 1 meV (at the edge of computational precision) with U^{Ni}=5 eV, reflecting a slight tendency toward FM ordering of the $4f$ moments. The energy difference between FM and AFM2 provides the difference between AFM and FM Ni moment alignment; AFM is favored by 116 (25) meV/Ni in GGA(+U). This energy difference contains information about Ni-Ni in-plane exchange coupling, and would give a value of the nearest neighbor coupling if more distant exchange couplings were negligible. Liu *et al.* have derived values of coupling for a few neighbors, concluding that the values depend strongly on the value of U^{Ni} that is assumed.[18]

For the FM bands shown in Fig. 1 the Ni and Nd moments are aligned into an overall FM structure. The Ni $d_{x^2-y^2}$ bands that give rise to the large FS are spin-split by 2 eV, reflecting the Ni spin moment of order $1\mu_B$. As noted earlier[4, 5] and recently by several others, Nd $5d$-derived bands dip below E_F at the zone center Γ and at the zone corner A, with bonding $5d_{z^2}$ and antibonding $5d_{xy}$ character respectively.[9] There is mixing with Ni d_{z^2} in both of these electron pockets, especially the latter. This mixing is due to the surprise that the minority (but occupied) Ni d_{z^2} antibonding band at $k_z = \pi$ (see the $Z-R-A-Z$ lines) lies within 0.2–0.4 eV of E_F.

As shown in Fig. 1, the $5d_{z^2}$ band energies relative to E_F of up (down) bands are –0.7 (+0.3) eV at Γ, giving an intra-atomic coupling $H^{Nd} = K\hat{e}_{4f}\cdot\hat{e}_{5d}$ with K=0.5 eV, in terms of the orientations of the $4f$ and $5d$ spins. For the antibonding $5d_{xy}$ orbital the eigenvalues at A lie at –1.2 eV with a splitting of less than 0.1 eV, reflecting the participation of Ni $3d$ orbitals and the out-of-phase character of states at the A point. Note that this coupling is Hund's rule alignment of $4f$ and $5d$ states and therefore anti-Kondo coupling of the local moment to the conduction band, as opposed to some suggested Kondo modeling of $Nd_{0.8}Sr_{0.2}NiO_2$.[4, 20] Such anti-Kondo coupling has been studied in other lanthanide compounds.[33] We return below to the $K \approx 0.5$ eV intra-atomic exchange coupling of Nd $5d$ states.

IV. NON-MAGNETIC Ni AND FERMI SURFACES

Low energy models of oxides including superconducting possibilities are based on non-magnetic Ni, with an on-site repulsion added to provide correlated electron behavior and a potential pairing mechanism. We have obtained a DFT+U solution with non-magnetic Ni (U_d^{Ni}=0, U_f^{Nd}=8 eV), our case AFM0. The Nd $4f$ moment that must remain fully spin-polarized has AFM alignment, so the Brillouin zone is correspondingly folded back. The Ni moment for AFM alignment is $1.2\mu_B$, compared to $1.0\mu_B$ for FM alignment. For U=0 (just GGA) the calculated moments $0.52\mu_B$ (AFM) and $0.35\mu_B$ (FM); *i.e.* there is

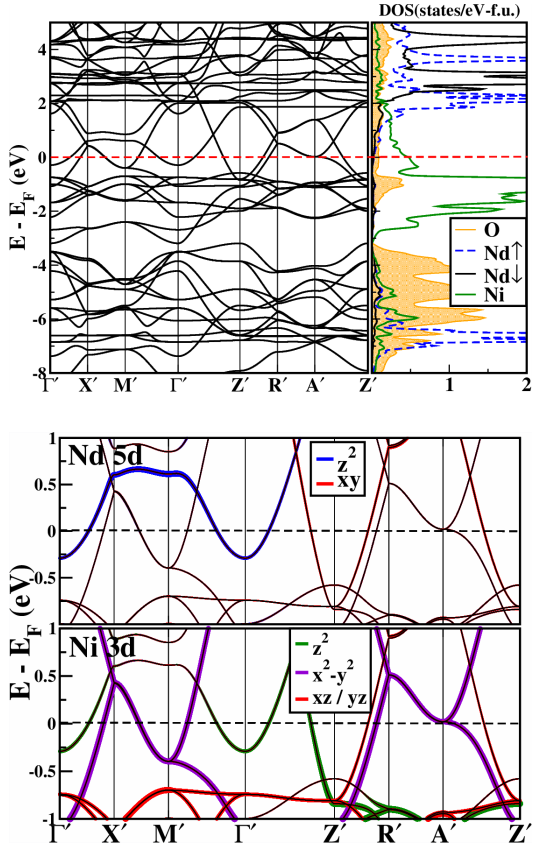

FIG. 2: Top: Bands of $NdNiO_2$, with AFM Nd moments and non-magnetic Ni layer, plotted along lines in the AFM zone. Bottom: Fatbands indicating Nd $5d$ character (above) and Ni $3d$ weight (below), with orbital character as noted. In terms of the usual NiO_2 sublattice, the $M(A)$ point is folded back to $\Gamma'(Z')$. The other symmetry points are $X' = (\pi/2, \pi/2, 0)$ and $M' = (\pi, 0, 0)$, while R' and A' lie above these points by $(0, 0, \pi)$ respectively.

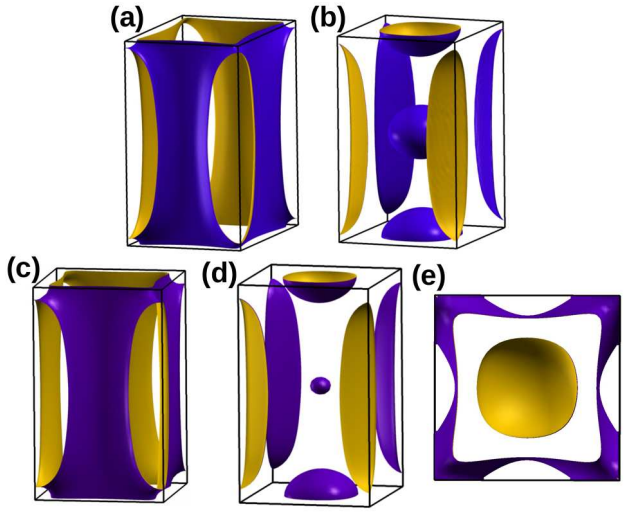

FIG. 3: Fermi surfaces for case AFM0 (non-magnetic Ni), in the full zone corresponding to AFM $4f$ alignment. Surfaces have been separated into left and right sub-panels for clarity. (a,b) undoped $NdNiO_2$. The spheres are (i) the Nd $5d$ electron pocket at $\Gamma' = \Gamma$, at the center of figure, and (ii) and the other electron pocket at A folded back to Z' (see text). (c,d): surfaces for VCA $Nd_{0.8}Sr_{0.2}NiO_2$, x=0.20 hole doping. The Γ-centered electron pocket is essentially emptied, while the Z'-centered pocket is almost unchanged. (e) Top view of the $Nd_{0.8}Sr_{0.2}NiO_2$ surfaces, showing the amount of k_z dispersion.

about $0.2\mu_B$ difference in the moments, and the associated Hund's energy would be an important contribution to the lower energies for AFM alignment.

The bands, density of states (DOS), and fatbands near E_F for AFM0 alignment are shown in Fig. 2, with symmetry points in that folded tetragonal zone now designated with primes. Gaps at the zone boundaries indicate effects of the Nd AFM order, *e.g.* a gap of 0.3 eV can be seen in the Nd $5d$ band around 0.8 eV at X'. As for the FM order above, this splitting vanishes for the corresponding antibonding band at R'. The nearby folded Ni $3d$ band displays no gap, reflecting canceling mixing with the eight neighboring Nd sites.

The bands crossing E_F giving the FSs are those that are fit to few band models. The corresponding FSs are shown in Fig. 3. The Nd $5d_{z^2}$ related electron pocket Pk1 at Γ has attracted attention, with the electron pocket Pk2 at A=(π, π, π) [Z' in Fig. 2] also receiving notice. Pk2 has strong Ni $3d_{z^2}$ character as well as some $3d_{xz,yz}$ influence, considerably stronger than the Nd $5d_{xy}$ component that has been discussed by several groups.[5–10] Due to k_z dispersion, the large Ni $d_{x^2-y^2}$ FS appears in this folded zone as a large banana centered at M', and strongly fluted cylinders also centered at M' and connected by tiny necks at the corner R' points. These two surfaces are degenerate along the zone faces reflecting simple folding back into the AFM zone, and correspond to M-centered hole barrels in the primitive zone that are familiar from cuprate physics. These barrels have surprisingly large k_z dispersion, lessening the relevance of two dimensional physics.

V. OCCUPIED $4f$ ORBITALS

We now consider briefly the Nd $4f$ contributions to the electronic and magnetic structure. The $S = \frac{3}{2}$ spin configuration is strongly enforced by Hund's first rule, and the energy difference between FM and AFM order of the Nd moments is very small, $\sim$ 7 meV/Nd ion for Ni treated in GGA, only 1 meV/Nd ion for Ni treated in GGA+U. The three occupied bands lie at –7 eV with some small dispersion due to the direct overlap of $4f$ and O $2p$ orbitals, which is small but provides crystal field splitting of the $4f$ orbitals. The occupied states that we obtained are combinations of $m_\ell = -3, -2, +1$, each with lesser admixtures of $+1, +2, -3$ states respectively, with total orbital moment m_{orb}=4.47 μ_B. When

spin-orbit coupling is included, the occupied orbitals are those with $j = \frac{5}{2}, m_j = -\frac{5}{2}, -\frac{3}{2}, +\frac{1}{2}$. (See SM for further information on these occupations.) The four unoccupied $4f$ bands are centered 3.5 eV above E_F but are spread by the anisotropy of the orbitals and mixing with Nd $5d$ states over a range of 3 eV.

VI. HOLE DOPING

$NdNiO_2$ becomes superconducting upon hole doping by 0.2 el/f.u.[1] With the Fermi level density of states N(0)=0.70/(eV cell), the drop in E_F (in rigid band) is 0.29 eV, which is enough to empty the Pk1 pocket at Γ to 0.4 eV, and to reduce the carrier density of Pk2 but leaving substantial Ni carriers. Rigid band treatment may be deceptive, however, due to Fermi level charge on both Ni and Nd atoms. We applied the virtual crystal approximation[34] (VCA) to obtain a more realistic effect of doping.

Fermi surfaces Pk1 and Pk2 of undoped [Fig. 3(a,b)] and x=0.20 doped $NdNiO_2$ [Fig. 3(c,d,e)] reveal important non-rigid band behavior, and the corresponding bands provided in Fig. 4 indicate the reason. The Ni d bands are shifted only slightly ($\sim$ 0.1 eV) with respect to E_F by doping, as is the band giving the A-centered pocket (at Z' in this figure). The Nd $5d$ band at Γ is however shifted by 0.3 eV and effectively emptied of its (undoped) 0.15 electrons. These VCA bands are similar to the VCA bands of Sakakibara *et al.*[7] for $La_{0.8}Ba_{0.2}NiO_2$, a difference being that their La $5d$ band is 0.2 eV higher than our Nd $5d$ band.

The band giving rise to Pk2, often referred to as Nd $5d_{xy}$, is also heavily Ni in character (shown above, and in the SM), hence little affected as are the other Ni $3d$ bands. The result is that $x = 0.20$ doping changes the Ni $3d$ charge by only 0.05 holes. The disappearance of pocket Pk1 and its associated disorder scattering may contribute to the drop in resistivity by a factor of 2–3 upon doping.[1]

VII. IMPLICATION OF SPIN DISORDER

The exchange splitting of the Nd $5d$ band at Γ (near E_F) reflects the intra-atomic $4f - 5d$ exchange on Nd of $K \approx 0.5$ eV. The $S = \frac{3}{2}$ spin moment on Nd drives this exchange splitting, which will follow the orientation of the $4f$ moment, which is disordered. With the very weak $4f - 4f$ exchange coupling noted in Sec. III, the Nd moments will be randomly oriented and quasi-static on an electronic time scale.

In spite of the disorder broadening on the electron Fermi pockets and resulting strong spin scattering driven by stable, essentially classical but disordered $4f$ moments, superconductivity survives in $Nd_{0.8}Sr_{0.2}NiO_2$. This situation bears some similarity to that of elemental Eu with its $4f^7$ moment: pressure kills magnetic order around 82 GPa but not the local moment, and there is a first order electronic but isostructural transformation to a superconducting phase at 1.7 K.[27] The exchange coupling from the classical local moment that should be disruptive to Cooper pairing in a specific spin configuration (singlet or triplet) may actually be contributing to the pairing in Eu.[28] The exchange coupling in $NdNiO_2$ is not as pervasive – every site in Eu has a $4f$ moment and the partially occupied conduction band is entirely $5d$ – but some of the physics may be related.

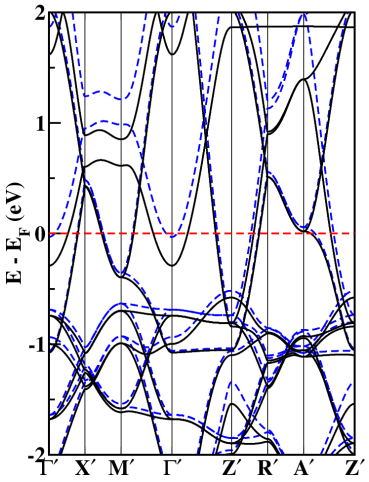

FIG. 4: Band structures of $Nd_{0.8}Sr_{0.2}NiO_2$ (dashed lines) compared to those of $NdNiO_2$ (solid lines), near E_F. Here $U_d^{Ni} = 0$; Ni is non-magnetic. The bands are plotted in the Nd AFM zone. Note that hole doping removes electrons primarily from the Γ-centered Nd $5f$ electron pocket; the Z' (A in primitive zone) pocket is nearly unchanged.

A related, and commonly modeled, spin-scattering process will occur on the (locally) magnetic Ni ion (as treated for the Cu ion in cuprates), an effect that can be modeled by any of a variety of spin fluctuation formalisms applicable to transition metal oxides. The resulting strong scattering in the electron pockets is a potential contributor to the resistivity of 'conducting' $NdNiO_2$, where the resistivity $\rho \sim 1m\Omega \cdot cm$ varies little between 300 K and the lowest temperature measured. The inferred mean free path in a Fermi liquid inspired Bloch-Boltzmann treatment would be atomic size, meaning incoherent transport and a washed out FS. A dynamical mean field approximation treatment of Ni $3d$ fluctuations[11] in $LaNiO_2$ found little shifting and broadening of bands around E_F, and no mechanism for the high resistivity. The large residual resistivity may be the result of the topotactic synthesis technique, with indications to be learned between the similarities and the distinctions between the doped thin films and doped bulk materials,[35] which also have similarly high residual resistivity.

VIII. SUMMARY

In this work we have focused on a primary distinction between $NdNiO_2$ and $LaNiO_2$. When the $4f$ moment on Nd is relegated to the core in nonmagnetic fashion, the electronic structures are nearly identical. Yet the Nd compound becomes superconducting while the sister La compound remains non-superconducting, when 20% hole-doped. We find that the strong Nd $4f$ moment is intra-atomic exchange-coupled to the Nd $5d$ orbitals by a coupling of roughly K=0.5 eV, giving anti-Kondo coupling between the Nd local moments and the lower conduction band. The disordered $4f$ moments will give rise to a broadening of $5d$ bands of the order of K, affecting transport and perhaps becoming implicated in pairing, either as a participant or a disruptive agent.

The calculated Ni moments are larger by $0.2\mu_B$ for antiferromagnetic alignment than for ferromagnetic alignment. The associated Hund's rule energy provides a tendency toward AFM alignment that lies beyond the usual Heisenberg exchange coupling picture. An important feature of this system is that the Γ-centered Nd $5d$ Fermi surface pocket accepts most of the doped holes, leaving Ni $3d$ charge changed only by 0.05 holes for 20% doping. The Pk2 spherical Fermi surface pocket that remains intact after doping, and rather strong k_z fluting of the Ni Fermi surfaces, suggests importance of k_z dispersion (three dimensionality). Our results indicate that several aspects of the Nd ion arising from the open $4f$ shell require attention for understanding both normal and superconducting state properties.

IX. ACKNOWLEDGMENTS

We acknowledge informative discussions with A. S. Botana, J. Sun, M. J. Han, E.-G. Moon, D. Lee, and J. Son, and communication with S. Raghu. M.Y.C. and K.W.L were supported by National Research Foundation of Korea Grants No. NRF-2019R1A2C1009588. W.E.P. was supported by NSF Grant DMR 1607139.

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