Tunable Kondo screening and interlayer hybridization effects in infinite-layer nickelates

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The discovery of superconducting nickelate compounds reignited the hope for elucidating the mechanism for high-$T_c$ superconductivity in the isostructural cuprate superconductors. In the cuprates, the superconducting gap opens up on a single-band of the quasi two-dimensional (2D) Fermi surface. On the contrary, the superconductivity of nickelates arises from a three-dimensional (3D) electronic structure with multi-band, implying significant interlayer electronic interactions. This raises an important question about the role of quasi-2D nature on the high-$T_c$ superconductivity and calls for a comprehensive investigation of the interlayer interactions in nickelates. Here, employing dynamical mean field theory, we show that Nd-4$f$ electrons in NdNiO$_2$ are strongly correlated with Ni-3$d$ giving rise to the Kondo effect and 3D nature of the electronic structure, unlike cuprates. We also found a significant interlayer hybridization between rare-earth-5$d$ and Ni-3$d$ electrons, resulting in the qualitatively different quasi-particle excitation from those in cuprates. Furthermore, we predict that the interlayer electronic interactions in nickelates can be suppressed by lattice modulation to achieve a quasi-2D electronic structure that promotes the occurrence of superconductivity.
Our findings naturally explain the recent experimental observations of appearance (absence) of superconductivity for the Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ film (bulk) with the large (small) $c$-axis lattice constant.

Recent reports on room temperature superconductivity in various hydrides under high pressure$^{1,2}$ promote another wave to search for high temperature superconductors at the ambient conditions. Although the observed high critical temperature ($T_c$) on superhydrides can be well explained by the conventional electron-phonon coupling mechanism$^{3,4}$, it requires the megabar pressure conditions to be stabilized. On the other hand, the mechanism of superconductivity through electronic channels has offered an alternative path to achieve a high-$T_c$ superconductivity. The copper-and iron-based superconductors are among the best examples where the intricate interaction between electron and low-energy bosonic excitation overcomes the Coulomb repulsion to form the Cooper pairs. Such a type of superconductivity requires strong electronic correlations and the sign-change in the superconducting energy gap, i.e. nodal superconductivity or sign-changing multi $s$-wave. An understanding of the electronic structure is of utmost importance.

A common thread in the electronic structures of these two families of copper-and iron-based superconductors is quasi-2D nature which provides a strong restriction on the possible pairing symmetries. Nevertheless, the discovery of nickelate superconductors$^5$ poses intriguing questions about the quasi-2D essence. In comparison with cuprates, whose Fermi surface displays the single-band of the Cu-$d$ and O-$p$ orbital characters$^{6,7}$, the nickelate’s Fermi surface consists of a Ni-$3d_{x^2−y^2}$ band and another mixed band including rare-earth-$5d$ $^{8−13}$. Despite that the nickelates have a
layered crystal structure, measured isotropic upper critical field reveals that the electronic structure
does not exhibit the quasi-2D behavior. On the contrary, Sun et al. showed the superconductivity in nickelates is anisotropic and it retains the quasi-2D picture. Theoretical study without considering lattice modulation suggested that doping can drive the multi-band nickelates into one-band Hubbard system, in agreement with monotonic increment of $R_H$-sign-change temperature with increasing doping level in Nd$_{1-x}$Sr$_x$NiO$_2$/SrTiO$_3$. Zeng et al., however, showed that negligible doping-dependence of $R_H$-sign-change temperature for $x \geq 0.23$ in La$_{1-x}$Ca$_x$NiO$_2$/SrTiO$_3$. Zeng et al. also pointed out the significant impact of lattice constant on the superconductivity in a variety of doped bulk and thin film nickelates. These controversial reports press a need for a thorough investigation of electronic interactions between NiO$_2$ and rare-earth layers and its variation under lattice modulation with a modern theory.

The discoveries of superconductivity in various rare-earth elements (La, Pr, Nd) nickelates suggest that superconductivity may not be influenced by the presence of 4$f$ electrons in the rare-earth layer. However, understanding the role of Nd-4$f$ in NdNiO$_2$, particularly at the vicinity of the Fermi level is an important and controversial subject from a theoretical point of view. By the dynamical mean field theory combined with density functional theory (DFT+DMFT), Liu et al. argued that the Nd-4$f$ electrons impact the electronic states far from the Fermi level, leading to unaffected electronic states close to the Fermi level. By DFT study, Choi et al. showed that an intra-atomic exchange coupling between the Nd-4$f$ spin and the Nd-5$d$ state in the magnetic ordered system can affect the state at the Fermi-level, and suggested anti-Kondo coupling of the local moment to the conduction bands. Non-negligible hybridization between Nd-4$f$ and Ni-3$d$
near the Fermi level was found in spin polarized simulations$^{21,22}$. Nevertheless, there is no sign of long-range magnetic ordering down to 1.7 K and 2.0 K for NdNiO$_2$$^{23}$ and LaNiO$_2$$^{24}$, respectively.

In this work, to ascertain the electronic structure of nickelates in paramagnetic normal state, we employ *ab-initio* many-body approach, dynamical mean field theory (DMFT) combined with linearized quasiparticle self-consistent GW (LQSGW) method. We found the Kondo screening of localized Nd-4$f$ by itinerant Ni-3$d$ and Nd-5$d$ in NdNiO$_2$, and strong interlayer hybridization between rare-earth-5$d$ and Ni-3$d$ in NdNiO$_2$ and LaNiO$_2$. It is shown that the both effects greatly affect the Fermi level, and can be fine-tuned by lattice modulation.

**Kondo effect in NdNiO$_2$.** Figure 1(a) shows crystal structure of tetragonal phase (P4/mmm) NdNiO$_2$, and the high symmetry lines in the first Brillouin Zone. The NiO$_2$-planers are separated by the Nd layer along the c-axis. Figure 1(b) shows spectral functions and density of states (DOS) of NdNiO$_2$ at $T = 100$ and 300 K. There are two notable differences between electronic structures at these two temperatures. First, DOS of Ni-3$d$ (green line) at around -1 eV at 100 K is larger than that at 300 K. This is attributed to interlayer hybridization effect and will be demonstrated in next section. Second, the DOS of Nd-4$f$ (red line) below the Fermi level at 300 K became sharp at 100 K. The flat Nd-4$f$ bands appeared at the Fermi level in the spectra function at 100 K. The flat $f$ bands hybridized with conducting $d$ bands giving rise to a kink-like band structure at the Fermi level along Γ-Z and R-A-Z, that is a hallmark of the Kondo screening$^{25}$. The calculated total occupation in Nd-4$f$ orbitals is 1.9 for both temperatures, indicating large local magnetic moment of Nd-4$f$ is screened by spin of conducting electrons at low temperature. This result is reminiscent
Figure 1: **Kondo effect in NdNiO$_2$.** (a) Layered crystal structure of NdNiO$_2$, and high symmetry lines in the first Brillouin Zone. (b) Calculated spectral functions and density of states at 100 K and 300 K. The red and green arrows indicate enhanced peaks at 100 K. (c) $d$ and $f$ orbitals are labelled and grouped for convenience in this work. Calculated electron occupation of Nd-4$f$ are presented. (d) Orbitals projected spectral functions at 300 K. Main orbital character at the vicinity of the Fermi level are denoted.

of heavy fermion superconductor UTe$_2$, where flat U-5$f$ bands with occupancy of 2.27 lead to orbital selective Kondo effect$^{25}$. For convenience in this work, $d$ orbitals are labelled, and grouped based on the main orbital character at the vicinity of the Fermi level as shown in Fig. 1(c). As shown in Fig. 1(d), Ni-$d_{\alpha}$, Ni-$d_{\beta}$, Nd-$d_{\alpha}$, and Nd-$d_{\beta}$ consist mainly of $x^2-y^2$, $z^2$, $xy$, and $z^2$ orbital, respectively. Ni-$d_{\alpha}$ is hybridized with Nd-$d_{\alpha}$ along the R-A-Z high symmetry line. Ni-$d_{\beta}$ is hybridized with Nd-$d_{\beta}$ along the $\Gamma$-X and M-R-Z high symmetry lines. We also group Nd-4$f$
orbitals into $f_\alpha$ and $f_\beta$ based on occupation. At $T = 300 \text{ K}$, Nd-$f_\alpha$ is hybridized with Nd-$d_\alpha$, Ni-$d_\alpha$, and Ni-$d_\beta$, whereas Nd-$f_\beta$ is hybridized with Nd-$d_\beta$ and Ni-$d_\beta$ at the vicinity of the Fermi level. At $T = 100 \text{ K}$, three Kondo scatterings appeared with momentum-dependent (see Fig. 1(b) and Fig. 2(b)): i) Nd-$f_\beta$ with Nd-$d_\alpha$, Ni-$d_\alpha$, and Ni-$d_\beta$ along R-A-Z, ii) Nd-$f_\beta$ with Nd-$d_\beta$ and Ni-$d_\beta$ at X and along M-Γ-Z, iii) Nd-$f_\alpha$ with Ni-$d_\alpha$ at X and near Γ point. This indicates that not only Nd-$5d$ but also Ni-$3d$ in NiO$_2$ layer are conducting electrons, which screen local spin momentum of Nd-$4f$.

Figure 2: **Kondo effect under lattice modulation.** (a) $T\chi_{\text{loc}}^{JZ}$ of Nd-$4f$ as a function of temperature in three lattices (mLC, rLC and pLC). (b) Orbitals projected spectral functions in the three lattices at 100 K. (c) Calculated density of states, the imaginary part of the self-energy on the imaginary and real frequency axis of Nd-$f_\alpha$ are presented. The temperature unit is K.
The Kondo effect, which manifests an interlayer interaction between localized Nd-4f and conducting Ni-3d, may depend on the distance between Ni and Nd. To investigate effect of lattice modulation on the Kondo screening, we adopted two experimental lattice constants of bulk NdNiO$_2$ and LaNiO$_2$ to build three inter-lattice constants. The one is experimental lattice constants of LaNiO$_2$ namely pLC, which is larger than regular experimental NdNiO$_2$ lattice constants (rLC). The smaller lattice constants (mLC) was built by reducing rLC by the lattice difference between pLC and rLC (see Fig. 2(a)). The difference between the lattices are \( \sim 0.04 \) and \( \sim 0.1 \) Å for in-plane and out-of-plane, respectively. The out-of-plane difference in the three lattices is close to \( c \)-axis monotonic increment from 3.28 Å to 3.42 Å upon zero to 25% Sr doping in Nd$_{1-x}$Sr$_x$NiO$_2$/SrTiO$_3$, and the shrinking from \( \sim 3.42 \) Å for the 4.6-nm film to \( \sim 3.36 \) Å for the 15.2-nm film of Nd$_{0.8}$Sr$_{0.2}$NiO$_2$/SrTiO$_3$. Note that there is no report on measured lattice constants under lattice modulation, and geometry optimization using many-body methods is not yet feasible. Here we emphasize that our choice of inter-lattice constants may not provide quantitative result. However, we expect to uncover some distinct features through such lattice modulation, by following some of the previous works, which produce electronic structures of nickelates using inter-lattice constants.

The Kondo effect is reduced as the lattice size increases, as indicated by weaker spectral weight of Nd-4f and diminishing band kinks at the Fermi level in the larger lattices (see Fig. 2(b)). The weaker Kondo effect in the larger lattices is also described by \( \chi_{\text{loc}}^{J_Z} \) of Nd-4f behavior in...
Fig. 2(a), where the local total angular momentum susceptibility is given as

$$\chi^J_{\text{loc}} = \int_0^\beta d\tau \langle J_z(\tau) J_z(0) \rangle.$$  \hspace{1cm} (1)

$\chi^J_{\text{loc}}$ of Nd-4$f$ in mL and rL deviates from the Curie-Weiss behaviors at $\sim$400 K indicating the onset of the Kondo scattering process\textsuperscript{25}. On the contrary, $\chi^J_{\text{loc}}$ of Nd-4$f$ in the pL keeps dropping with lowering temperature, which indicates undetectable Kondo screening effect\textsuperscript{25}.

To understand the diminishing Kondo effect in the larger lattices, we calculated the self-energy as shown in Fig. 2(c). The self-energies of Nd-$f_\alpha$ on the imaginary frequency axis at 900 K in the three lattices exhibit a singularity, which indicates that the electronic structure at high temperature is governed by Mott-like physics. This leads to formation of strong self-energy peak at the Fermi-level on the real frequency axis and appearance of a gap in the DOS. At a lower temperature, the self-energy exhibits Fermi-liquid-like behavior giving rise to a formation of quasiparticle peak at the vicinity of the Fermi level. The Mott-like feature is more pronounced in the larger lattices owing to suppressed inter-orbital hopping, which is manifested by smaller hybridization function, as shown in Supplementary Fig. S2. The prominent Mott-like characteristic of Nd-4$f$ in the larger lattices hinders the formation of quasiparticle peak at the Fermi level, resulting in less Kondo effect. Our results are reminiscent of Fermi-liquid behavior of 5$f_{5/2}$ states with larger Kondo scale than the 5$f_{7/2}$ states which are at the edge of a Mott transition in PuCoGa\textsubscript{5}\textsuperscript{31}. Interestingly, the two features are competing in the same states of NdNiO\textsubscript{2}.

The Kondo effect in NdNiO\textsubscript{2} without implementing Nd-4$f$ has been proposed\textsuperscript{5,32–34}. While spin momentum of Ni-3$d_{x^2−y^2}$ is screened by other conducting $d$ or interstitial-$s$ electrons in those
works, our results apparently show that Nd-4\textit{f} is essentially a heavy fermion giving rise to Kondo effect at low temperature. We do not provide quantitative Kondo scaling temperature, which is comparable with measures of electrical resistivity. Instead, based upon our findings, we propose that Kondo temperature is lattice dependent. There is a resistivity upturn at \(\sim 70\) K for NdNiO\textsubscript{2} film (\(c\)-axis lattice constant: 3.31 Å)\textsuperscript{5}, whereas insulating resistivity behavior arises below 300 K in NdNiO\textsubscript{2} bulk (\(c\)-axis lattice constant: 3.24 Å)\textsuperscript{35}. While the Kondo effect is not the only possibility for the resistivity upturn, these observations could indicate higher onset temperature of Kondo scattering in NdNiO\textsubscript{2} bulk than film, and be tied to our result of weaker Kondo effect in larger lattice.

**Interlayer hybridization in LaNiO\textsubscript{2} and NdNiO\textsubscript{2}**. LaNiO\textsubscript{2} has the same crystal structure as NdNiO\textsubscript{2}, and La-4\textit{f} states are far away from the Fermi level. To investigate aforementioned interlayer hybridization effect in NdNiO\textsubscript{2}, we first calculated the electronic structure of LaNiO\textsubscript{2}, for the sake of simplicity. The two left panels of Fig. 3(b) show DOS of Ni-\(d_\alpha\) and La-\(d_\beta\). The interlayer hybridization effect is manifested through the same evolution of Ni-\(d_\alpha\) and La-\(d_\beta\) peaks at \(\sim -1.0\) eV with lowering temperature. The peaks are absent at 2000 K, and developed along the X-M-R symmetry line with lowering temperature as shown in Fig. 3(a). Since Ni-\(d_\alpha\) is hybridized with O-2\textit{p} near the peak, the peaks positions are slightly different. The apparent coincidence of peak positions of Ni-3\textit{d} and La-5\textit{d} is presented by one orbital projected DOS in Supplementary Fig. S3. Due to formation of the peaks, Ni-\(d_\alpha\) peak at the Fermi level shifted to lower energy with lowering temperature, as shown in the right top panel of Fig. 3(b). The shift alters DOS at the Fermi level, and naturally impacts a quasi-particle excitation.
Figure 3: **Temperature evolution of interlayer hybridization effect.** (a) Ni-\(d_\alpha\) and La-\(d_\beta\) projected spectral functions at 100, 600, 1000 and 2000 K. (b) Ni-\(d_\alpha\), La-\(d_\beta\), Ni-\(d_\alpha\) and Ni-\(d_\beta\) projected density of states. The simulation temperature unit is K. The blue arrows denote the evolution of peaks of Ni-\(d_\alpha\) and La-\(d_\beta\) with lowering temperature. (c) \(D(i\omega_0)\) (solid lines) of Ni-\((d_\alpha,d_\beta)\) and Nd-\((f_\alpha,f_\beta)\), and \(\chi^{JZ}_{loc}\) (dashed lines) of Ni-3\(d\) in three lattices of pLC (blue), rLC (red) and mLC (green) for LaNiO\(_2\) and NdNiO\(_2\).

The interlayer hybridization is established by the interaction between Ni-\(d_\alpha\) and La-\(d_\beta\), and may depend on the distance between Ni and La. To investigate effect of lattice modulation on the interlayer hybridization, like NdNiO\(_2\), three inter-lattices (mLC, rLC, and pLC) are built, where rLC is experimental lattice parameters for LaNiO\(_2\) (see Fig. 3(c)). Fig. 3(c) shows DOS at the Fermi level, which is determined by

\[
D(i\omega_0) = -\frac{1}{\pi} \text{Im}G(i\omega_0)
\]
where \( \omega_0 \) is the first Matsubara frequency and \( G \) is the calculated local Green’s function. \( D(i\omega_0) \) of Ni-\( d_\beta \), which is hybridized with La-\( d_\beta \) at the vicinity of the Fermi level are almost the same in magnitude with identical temperature dependence in the three lattices. This indicates a negligible effect of lattice modulation. All DOS of Ni-\( d_\beta \) at the Fermi level are gradually increased with lowering temperature (see also the right bottom panel of Fig. 3(b)). This behavior is reminiscent of evolution of quasiparticle peaks in strongly correlated materials where the spectral weight at the Fermi level is transferred from the upper and lower Hubbard bands \(^{25,36,37}\). On the contrary, \( D(i\omega_0) \) of Ni-\( d_\alpha \) is larger in the larger lattices in all temperature ranges (\(< 1000 \) K). They exhibit a broad downturn at \( T > 1000, \sim 900 \) and \( \sim 700 \) K for mLC, rLC and pLC, respectively. The Ni-\( d_\alpha \) and La-\( d_\beta \) peaks are weakened and shifted to higher energy in the larger lattices as shown in Supplementary Fig. 3 and 4, indicating weaker interlayer hybridization effect in the larger lattices. \( \chi_{J_z}^{J_g} \) of Ni-3\( d \) in the three lattices gradually decreased with lowering temperature. The deviation from the Curie-Weiss behaviors indicates significant screening of local total angular momentum of Ni-3\( d \). More suppressed \( \chi_{J_z}^{J_g} \) of Ni-\( d \) in the smaller lattices indicates stronger screening effect. These results imply that quasi-particle excitation of Ni-\( d_\alpha \) is greatly affected by the lattice modulation, and associated with the interlayer hybridization effect.

The origin of the effect of lattice modulation on interlayer hybridization can be identified with the self-energy which captures interaction between electron and surrounding medium, and hybridization function which describes electron hopping. Whereas variations in DOS, self-energy and hybridization function of Ni-\( d_\beta \) as a function of temperature are minor (see Supplementary Fig. S5), the drastic changes in DOS and self-energy peaks of Ni-\( d_\alpha \) are manifested in the three
lattices, as shown in Supplementary Fig. S6. The self-energy peak is weakened and dropped rapidly in the larger lattices. In consequence, the Ni-$d_\alpha$ peaks are smaller in the larger lattices and decrease faster with increasing temperature. Reducing lattice constants, particularly along the $c$-axis, enhances interlayer hybridization between Ni-$d_\alpha$ and La-$d_\beta$. As shown in Supplementary Fig. S6, there are three major peaks in the hybridization function. While the first peak from the Fermi level hybridized mainly with O-$2p$, other peaks hybridized with sizable La-$5d$. The central peak at $\sim -6$ eV can represent the hybridization channel between Ni-$d_\alpha$ and La-$d_\beta$. As shown in Supplementary Fig. S7, the central peak of hybridization function is slightly enhanced with its lower energy level in the smaller lattices. These results indicate that stronger hybridization in the smaller lattices lead to enhanced self-energy and a pronounced interlayer hybridization effect.

We illustrate our results in the Supplementary Information (Supplementary Fig. S8, S9 and S10) to show substantial interlayer hybridization effect in NdNiO$_2$. The interlayer hybridization effect in NdNiO$_2$ is manifested in the same fashion as in LaNiO$_2$ down to $\sim 200$ K, below which the Kondo effect is substantiated by increased $D(i\omega_0)$ of Ni-$3d$ and Nd-$4f$ (see Fig. 3 (c)). The interlayer hybridization peaks of Ni-$d_\alpha$ and Nd-$d_\beta$ are more pronounced in smaller lattices (mLC > rLC > pLC). As shown in Fig. 3 (c), $D(i\omega_0)$ of Ni-$d_\alpha$,$d_\beta$ and $\chi_{\text{loc}}^{Jz}$ of Ni-$3d$ for both LaNiO$_2$ and NdNiO$_2$ followed the same trend with respect to the lattice modulations. In comparison to LaNiO$_2$, one notable difference in NdNiO$_2$ is that onset temperatures of interlayer hybridization effect, which is approximately determined by peak position of $D(i\omega_0)$ and $\chi_{\text{loc}}^{Jz}$ of Ni-$3d$, are relatively lower than that of LaNiO$_2$. This indicates weaker interlayer hybridization effect in NdNiO$_2$, which is attributed to weaker hybridization function. As shown in Supplementary Fig. S7 and S11, the
hybridization function peaks (central peaks) for the three lattices are lower and at higher energy in NdNiO$_2$ in comparison to that in LaNiO$_2$. The other notable difference is that the first hybridization function peak at $\sim -5$ eV change drastically in NdNiO$_2$ indicating stronger hybridization between Ni-$3d$ and O-$2p$ (see Supplementary Fig S6 and S10).

**Suggestive effect of lattice modulation on superconductivity.** We have shown Kondo screening and interlayer hybridization effects raised by interaction between NiO$_2$ and rare-earth layers. This imply 3D electronic structure in bulk parent nickelates, unlike cuprators, where quasi-

Figure 4: Schematic diagram of suppressing interlayer interaction effects. Schematic diagram illustrates interrelationship among the strong electronic interaction, dimensionality, and high-$T_c$ superconductivity in doped NdNiO$_2$. Doping and increasing lattice size can suppress the interlayer interactions leading to the quasi-2D single-band feature, which is essential for the superconductivity.
2D symmetry is essential for high-$T_c$ superconductivity\textsuperscript{38}. The recent measure of significant angle-dependent $T_c$, however, emphasizes a more important role of quasi-2D bands comprised of Ni-$3d_{x^2−y^2}$ than the 3D electron bands in pairing formations in nickelates\textsuperscript{15}. We suggest that the 3D electronic structure of NdNiO$_2$ can be fine-tuned in favor of the quasi-2D electronic structure by hole doping and lattice modulation.

The Fermi surface of NdNiO$_2$ consists of multi-band: the Ni-$d_\alpha$ band and mixed band of Nd-$d_\beta$, Ni-$d_\beta$ and Nd-$d_\alpha$. The latter is so-called self-doping band, which can be lifted from the Fermi level by hole doping leading to increased carrier and a single-band feature\textsuperscript{8,30}. According to our results, the single-band is subject to interlayer interactions (Kondo screening and hybridization effects) in the regular lattice. Increasing lattice size can suppress the interlayer interactions leading to the quasi-2D feature, which is essential for the high-$T_c$ superconductivity, as schematically shown in Fig. 4. Our findings can be linked to following three experimental observations of appearance (absence) of superconductivity for the Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ film (bulk) with the large (small) $c$-axis lattice constant. First, the hole doping arise lattice modulation of $c$-axis monotonic increment from 3.28 Å to 3.42 Å upon zero to 25\% Sr doping in Nd$_{1−x}$Sr$_x$NiO$_2$/SrTiO$_3$ thin films, where superconducting dome appear for $0.125 < x < 0.25$\textsuperscript{27}. The $c$-axis lattice constant is $\sim$3.38 Å for Nd$_{0.8}$Sr$_{0.2}$NiO$_2$/SrTiO$_3$. Second, the superconductivity is observed in films with thickness ($c$-axis lattice constant) ranging from 4.6-nm ($\sim$3.42 Å) to 15.2-nm ($\sim$3.36 Å) in Nd$_{0.8}$Sr$_{0.2}$NiO$_2$/SrTiO$_3$\textsuperscript{28}. Third, no superconductivity is observed in Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ bulk\textsuperscript{35}. Its $c$-axis lattice constant is 3.33 Å, which is smaller than that of the films.
Methods

We use *ab-initio* linearized quasiparticle self-consistent GW (LQSGW) and dynamical mean field theory (DMFT) method \(^{39–41}\) to calculated the electronic structure of LaNiO\(_2\) and NdNiO\(_2\) which crystallizes into tetragonal space group P4/mmm (No. 123) \(^{23,26}\). The LQSGW+DMFT is designed as a simplified version of the full GW+EDMFT approach \(^{42–44}\). It calculates electronic structure by using LQSGW approaches \(^{45,46}\). Then, it corrects the local part of GW self-energy within DMFT \(^{47–49}\). We adopted experimental lattice constants of \(a = 3.96\) and \(c = 3.38\) Å \(^{26}\) and \(a = 3.92\) and \(c = 3.28\) Å \(^{23}\) for LaNiO\(_2\) and NdNiO\(_2\), respectively. Using the two lattice constants, we create inter-lattice parameters to model lattice modulation. Other than the lattice parameters, we explicitly calculate all quantities such as frequency-dependent Coulomb interaction tensor and double-counting energy. Then, local self-energies for Ni-3\(d\) and Nd-4\(f\) are obtained by solving two different single impurity models. La-5\(d\) and Nd-5\(d\) are treated within GW approximation. Test simulations, which treat rare-earth-5\(d\) as strongly correlated orbitals within DMFT, show qualitatively similar Kondo effect (kink-like band structure at the Fermi level along Γ-Z) and inter-layer hybridization effect (data are not presented) with presented results. Spin-orbital coupling is included for all calculations. For the details of method, please see the supplementary methods.

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Author contributions  B.K. designed the project. B.K., H.K. and Q.Z. wrote the manuscript. B.K. performed the calculations and conducted the data analysis. All authors discussed the results and commented on the paper.

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