Core-Level X-Ray Spectroscopy of Infinite-Layer Nickelate: LDA+DMFT Study

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(Dated: October 26, 2021)

Motivated by recent core-level x-ray photoemission spectroscopy, x-ray absorption spectroscopy (XAS), and resonant inelastic x-ray scattering (RIXS) experiments for the newly discovered superconducting infinite-layer nickelate, we investigate the core-level spectra of the parent compounds NdNiO2 and LaNiO2 using the combination of local density approximation and dynamical mean-field theory (LDA+DMFT). Adjusting a charge-transfer energy to match the experimental spectra, we determine the optimal model parameters and discuss the nature of the NdNiO2 ground state. We find that self-doping from the Nd 5d states in the vicinity of the Fermi energy prohibits opening of a Mott-Hubbard gap in NdNiO2. The present Ni L3 XAS and RIXS calculation for LaNiO2 cannot explain the difference from NdNiO2 spectra.

I. INTRODUCTION

High-\(T_c\) superconductivity of cuprates has been a focal point of 3d transition-metal oxide (TMO) physics over the past 30 years [1–3]: nevertheless, the underlying mechanism remains elusive. Superconductivity [4] reported recently in layered nickelate Nd0.8Sr0.2NiO2 (\(T_c = 9–15\) K) with a similar crystal structure may provide new clues. The fundamental question is whether the electronic structure of NdNiO2 (and LaNiO2) is similar to that of high-\(T_c\) cuprates. Naively, one might presume that Ni in the undoped systems is monovalent and, thus, hosts the \(d^8 (S = 1/2)\) ground state similar to cuprates. However, theoretical studies [5–9] suggest a self-doping from Nd (or La) 5d orbitals. Additionally, holes doped to a low-valence Ni\(^{1+}\) compound may reside in Ni 3d orbitals, unlike in cuprates [2, 3, 10] or NiO with Ni\(^{2+}\) [11], where they occupy the O 2p states.

The Ni 2p3/2 core-level x-ray photoemission spectroscopy (XPS) [12], x-ray absorption spectroscopy (XAS), and resonant inelastic x-ray scattering (RIXS) [9, 13] are employed to probe the electronic structure of infinite-layer nickelates. A shoulder observed in the main line of the Ni 2p1/2 XPS spectra in NdNiO2 [12] is attributed to Ni-Ni charge-transfer (CT) response to the creation of the core hole, a process traditionally called nonlocal screening (NLS) [14]. Generally, NLS provides valuable information about the electronic structure of TMOs [15–18]. For high-\(T_c\) cuprates, the NLS in Cu 2p3/2 XPS is extensively used to determine key parameters, such as the CT energy \(\Delta_{\text{ep}}\), and more recently to analyze electronic reconstructions due to doping [19–24].

Further information can be obtained with charge-conserving spectroscopies XAS and RIXS. The Ni L3 edge XAS and RIXS spectra are measured in both NdNiO2 [9, 13] and LaNiO2 [9]. Interestingly, a side peak (852.0 eV) is observed in L3-XAS of LaNiO2, while it is absent in NdNiO2. A low-energy RIXS feature \((E_{\text{loss}}=0.6\) eV) associated with the XAS side peak is observed in LaNiO2. The difference between the Ni L3 XAS and RIXS spectra of NdNiO2 and LaNiO2 poses an open question.

In this paper, we use the local-density approximation (LDA) + dynamical mean-field theory (DMFT) [24–26] to calculate XPS, XAS, and RIXS spectra [16, 27–30] of undoped infinite-layer nickelates. By comparison with the available experimental data, we identify the most appropriate CT energy and use it for classification within the Zaanen-Sawatzky-Allen scheme [10].

Material-specific DMFT calculations for NdNiO2 or LaNiO2 were performed by several authors, leading to contradictory conclusions, which can be sorted into two groups: (i) Multiorbital (Hund’s metal) physics is crucial [31–34], and (ii) (single-orbital) Mott-Hubbard physics is relevant with little influence of charge-transfer effects or with a small self-doping by Nd 5d electrons [35–37]. The differences, recently addressed blueb yKarp, Hampel, and Millis [38], can be traced to the model parameters, which are not uniquely defined, such as the interaction strength, orbital basis, and, in particular, the double-counting correction. To settle the debate, an experimental input is needed to provide a benchmark for selecting the model parameters.

II. COMPUTATIONAL METHOD

The XPS, XAS and RIXS simulations start with a standard LDA+DMFT calculation [16, 25–28, 39]. First, LDA bands for the experimental crystal structure of NdNiO2 and LaNiO2 [40] are calculated using the Wien2K package [41, 42] and projected onto Wannier basis spanning the Ni 3d, O 2p, and Nd (La) 5d orbitals [43, 44]. The model is augmented with a local electron-electron interaction within the Ni 3d shell, parametrized by Coulomb’s \(U=5.0\) eV and Hund’s \(J=1.0\) eV [31, 32, 45]. The strong-coupling continuous-time quantum Monte Carlo impurity solver [46, 49] is employed with the DMFT cycle to obtain the Ni 3d self-energy \(\Sigma(i\omega_n)\), which is analytically continued to real frequency after having reached the self-consistency.
calculations are performed at temperature $T = 290$ K.

The XPS, XAS, and RIXS spectra are calculated from the Anderson impurity model augmented with the 2$p$ core states and the real-frequency hybridization function discretized into 40–50 levels (per spin and orbital). To this end, we use the configuration-interaction solver; for details, see Refs. 16 and 29 for XPS and Refs. 27, 28, and 51 for XAS and RIXS simulation.

Determination of Ni 3$d$ site energies in the model studied by DMFT involves subtracting the so-called double-counting correction $\mu_{dc}$ from the respective LDA values ($\varepsilon_d^{LDA}$), a procedure accounting for the effect of the $dd$ interaction present in the LDA description. It is clear that $\mu_{dc}$ is of the order of Hartree energy $U n_d$, but a generally accepted universal expression is not available [20, 52, 53] for NdNiO$_2$-specific discussion. Variation of $\mu_{dc}$, on the other hand, may have a profound effect. Therefore we choose to adjust $\mu_{dc}$ by comparison to the experimental data. Although $\mu_{dc}$ is the parameter entering the calculation, in the discussion we use its linear function $\Delta_{dp} = (\varepsilon_d^{LDA} - \mu_{dc}) + 9 U_{dd} - \varepsilon_p^{LDA}$, which sets the scale for the energy necessary to transfer an electron from O 2$p$ to Ni 3$d$ orbital. Here, $U_{dd} = U - \frac{4}{3} J$ is the average interorbital interaction, and 9 is the Ni 3$d$ occupation in the Ni$^{2+}$ formal valence (similar to the definition of the charge-transfer energy in the cluster model [28, 29, 55]).

**III. ELECTRONIC STRUCTURE**

Figure 1 shows the orbitally resolved spectral densities (projected density of states) of NdNiO$_2$ obtained by LDA and LDA+DMFT for $\Delta_{dp} = 4.9$ eV, which we later identify as the optimal parameter choice. Both the LDA and LDA+DMFT yield a metallic state with the Ni $x^2-y^2$ orbital character dominating around the Fermi level. This general picture is valid in the entire range of studied $\Delta_{dp} = 2.9–6.9$ eV. In Fig. 2 we show the dependence of Ni $x^2-y^2$ and $3z^2-r^2$ spectra on $\Delta_{dp}$. Increasing $\Delta_{dp}$ corresponds to an upward shift of the bare Ni 3$d$ site energies, which is indirectly reflected in the shift of the $3z^2-r^2$ band. The $x^2-y^2$ peak at the Fermi level, rather than being shifted, exhibits an increased mass renormalization (reduced width). The amplitude of the $x^2-y^2$ hybridization function around the Fermi level is reduced with increasing $\Delta_{dp}$; in particular, the sizable decrease just below the Fermi level (blue region) has an important implication for the XPS spectra as discussed later. The evolution of $x^2-y^2$ and $3z^2-r^2$ occupancies in Fig. 4 shows that, up to $\Delta_{dp} \approx 7$ eV the $3z^2-r^2$ is completely filled (the deviation from 2.0 is due to hybridization with empty bands). The physics is, thus, effectively of a single-orbital Hubbard model, and the Ni ion takes a monovalent ($\text{Ni}^{1+}$, $d^0$) character.

Different from cuprates, the stoichiometric parent compound is metallic. In order to analyze the role of Nd $d$ bands, we study two modified models: (i) hybridization between NiO$_2$ planes and the Nd orbitals is switched off, and (ii) Nd orbitals are removed from the model. In the
former case (i) self-doping of the NiO$_2$ planes from Nd orbitals is possible, while in the latter case (ii) the stoichiometry of the NiO$_2$ planes cannot change. The evolution of the $x^2-y^2$ spectral density with $\Delta_{dp}$ for (i) and (ii) is shown in Fig. 3. Like the full model, the low-energy spectrum of model (i) remains metallic over the whole studied range of $\Delta_{dp}$. Removing the Nd orbitals (ii) results in progressive mass renormalization with increasing $\Delta_{dp}$ and eventually opening of a gap above $\Delta_{dp} = 5.9$ eV. This can be understood as a result of effective weakening of the Ni-O hybridization, i.e., a bandwidth-driven Mott transition. The NiO$_2$ layers in NdNiO$_2$ can, thus, be viewed as a strongly correlated system in the vicinity of Mott transition, where the insulating state is precluded by the presence of Nd 5$d$ bands [56].

IV. COMPARISON TO EXPERIMENTAL X-RAY SPECTROSCOPIES

A. Ni 2$p_{3/2}$ XPS

Next, we investigate the impact of the variation of $\Delta_{dp}$ on the core-level spectra. Figure 3 shows the calculated Ni 2$p_{3/2}$ XPS spectra of NdNiO$_2$ together with the experimental data [12]. The Ni 2$p_{3/2}$ XPS spectrum consists of two components: the main-line (852–857 eV) and the CT satellite (861 eV) [16, 55]. The core hole created by x rays represents an attractive potential, which induces CT from surrounding atoms to the empty 3$d$ orbital on the excited Ni site. The main line corresponds to the CT screened final states, while the CT satellite corresponds to unscreened ones [14, 16, 29]. Fu et al. [12] observe a shoulder B (approximately 856.5 eV) in the main line. Unlike A, the peak B is absent in the cluster-model spectra [14, 29] and, thus, can be ascribed to NLS [12]. The sensitivity of the relative intensity of A and B to $\Delta_{dp}$ can be used to locate its value to the interval 4.9–5.9 eV. The observed behavior of the NLS feature B reflects the amplitude of the hybridization function just below the Fermi level [10], the shaded area in Fig. 2(c).

The NLS (B) is known to dominate over the local screening (A) in cuprates, as shown in Fig. 3 for Cu 2$p_{3/2}$ XPS in La$_2$CuO$_4$ [19]. For small $\Delta_{dp} = 2.9$ eV, a typical value for high-$T_c$ cuprates [10, 14, 19, 23, 57], the spectra of NdNiO$_2$ resemble that of La$_2$CuO$_4$. Thus our analysis shows that $\Delta_{dp}$ in NdNiO$_2$ is by 2–3 eV larger than in cuprates. The relative size $\Delta_{dp}$ and the Hubbard $U$ would place NdNiO$_2$ somewhere between the Mott-Hubbard ($\Delta_{dp} > U$) and CT ($\Delta_{dp} < U$) systems in the Zaanen-Sawatzky-Allen classification of TMOs [10, 37, 58, 59]. The calculated occupations for doped Nd$_{0.775}$Sr$_{0.225}$NiO$_2$, shown in Fig. 4 and in Supplementary Material [54], reveal that for optimal $\Delta_{dp}$ doped holes are almost equally shared by Ni, Nd and O sites. This is a remarkable difference to monovalent cuprates or divalent NiO. In these systems of strong charge-transfer character, the doped holes reside predominantly in O 2$p$ orbitals, irrespective of a substantial 3$d$ spectral weight just below the Fermi level [60]. Moreover, for the optimal $\Delta_{dp}$ values inferred above, the doped holes in NiO$_2$ do not enter the Ni 3$p^2 - r^2$ orbitals (Fig. 1). The single-band Hubbard description is thus valid for not only the parent NdNiO$_2$ but also the superconducting one Nd$_{0.8}$Sr$_{0.2}$NiO$_2$, as suggested by Refs. [33, 37].

Proximity to NiO$_2$ layers to a Mott state (precluded by self-doping from Nd) suggests that a superexchange interaction still plays a role despite the metallic state. Using the optimal $\Delta_{dp}$ we arrive [54] at the nearest Ni-
FIG. 5. (a) Ni 2p3/2 XPS spectra and (b) Ni 2p3/2 XAS spectra of NdNiO2 calculated by the LDA+DMFT method for different Δdp values. The experimental data [9, 12] are shown together. For comparison, experimental Cu 2p3/2 XPS data of La2CuO4 are shown (gray) [19]. The spectral broadening is taken into account using a Lorentzian 300 meV (HWHM) and a Gaussian 250 meV (HWHM) for XAS and a Lorentzian 500 meV and a Gaussian 400 meV for XPS. The XPS spectra with different broadening widths can be found in Supplemental Material [54].

Ni anti-ferromagnetic exchange in the range 40–60 meV. Given the oversimplification of representing spin response of a metal in terms of local moments interactions, this value is consistent with 69 meV inferred from the RIXS experiment on a related compound La4Ni3O8 [61].

The calculated LaNiO2 spectra in Fig. 6(a) show similar behavior to NdNiO2.

B. Ni 2p3/2 XAS and RIXS

As expected for Ni1+ systems with a d9 configuration, the experimental Ni 2p3/2 XAS of NdNiO2 shows a sharp peak corresponding to the electron excitation from the 2p3/2 to an empty x2 − y2 orbital [Fig. 5(b)]. The XAS main peak is accompanied by a broad tail attributed to the hybridization with metallic bands. The theoretical results in Fig. 5(b) reproduce the experimental data reasonably well; however, the weak dependence on Δdp does not allow to draw conclusions about its value.

The RIXS spectra, on the other hand, exhibit fine changes with the Δdp values, see Fig. 7. The spectra at all Δdp values contain a strong Raman-like (RL) feature (at constant E_loss irrespective of the incident photon energies E_in) at E_loss ~1 eV and a fluorescence-like (FL) feature (E_loss linearly increases with E_in). The RL feature arises from t2g → x2 − y2 excitation, and its width (in E_loss) reflects a rapid decay of this local “exciton”. With increasing Δdp, the RL feature shifts to lower energies, due to an upward shift to the t2g bands similar to 3z2 − r2 shown in Fig. 2(b), while the x2 − y2 peaks remain pinned in the vicinity of the Fermi level. The main variation of the RIXS spectra with increasing Δdp concerns the behavior of the FL part, the onset of which is pushed to higher E_loss. For Δdp = 4.9 eV, deduced from the XPS data, the FL feature sets in below the RL feature at around E_loss ~0.6 eV. The coexisting RL and FL features above well capture the experimental data by Hepting et al. [9] and Rossi et al. [13]. Artificial suppression of hybridization to Nd 5d states [Fig. 7(c)] leads to a reduced intensity of the FL feature and only a moderate modification of the low-energy spectra supporting the conclusion about the electron-reservoir role of Nd 5d states.

Finally we discuss XAS and RIXS spectra in LaNiO2 (the experimental XPS data are not available at the moment). The experimental XAS spectra of LaNiO2 [9] are clearly distinct from NdNiO2. A side peak at 852.0 eV is attributed to Ni-La hybridization effect by Hepting et al. [9] based on a simplified impurity model simulation. The LDA+DMFT calculations (including Ni-La hybridization) do not support this conclusion as they do
FIG. 7. The Ni $L_3$ RIXS spectra of NdNiO$_2$ calculated for (a) $\Delta_{dp} = 3.9$ eV, (b) $\Delta_{dp} = 4.9$ eV, (c) $\Delta_{dp} = 5.9$ eV, and (d) $\Delta_{dp} = 6.9$ eV. (e) the Ni $L_3$ RIXS spectra calculated for the model without the hybridization between Nd 5$d$ and NiO$_2$ plane ($\Delta_{dp}=4.9$ eV). The spectral broadening is considered using a Gaussian of 100 meV (HWHM).

not match the experimental XAS spectra. While large $\Delta_{dp}$ gives rise to a high-energy XAS shoulder (Fig. 6), it does not improve the agreement of the RIXS spectra, shown in Fig. 8. We have to conclude that the present LDA+DMFT description of LaNiO$_2$ does not match the experiment for any choice of $\Delta_{dp}$.

We propose that the problem lies on the experimental side; i.e., the measured spectra do not represent a perfect LaNiO$_2$ crystal. We argue by the success of the present method for a broad spectrum of transition-metal oxides [16] including NdNiO$_2$ as well as the absence of an obvious source of difference between NdNiO$_2$ and LaNiO$_2$. On the experimental side, we point out recent studies [12, 13] reporting superconductivity in Sr-doped LaNiO$_2$, suggesting that NdNiO$_2$ and LaNiO$_2$ are not that different after all. Spectroscopic experiments on these new LaNiO$_2$ samples are needed to resolve the present discrepancy.

V. CONCLUSIONS

We have presented a comprehensive analysis of Ni 2$p_{3/2}$ core-level XPS, XAS, and RIXS in infinite-layer nickelates (NdNiO$_2$ and LaNiO$_2$) with the LDA+DMFT approach. Comparison to the experimental spectra allowed us to determine the CT parameter (double-counting correction) and make the following conclusions about the electronic structure. Undoped NdNiO$_2$ is nearly monovalent (Ni$^{4+}$, $d^8$) with a small self-doping from the Nd 5$d$ band. Only the Ni $x^2−y^2$ orbitals are partially filled and multiorbital physics does not play an important role for the stoichiometric as well as slightly hole-doped compound. Unlike in cuprates, the Ni-O hybridization does not play an important role in connection with doping – doped holes reside predominantly on the Ni sites. The physics of NdNiO$_2$ described effectively by a single-band Hubbard model [35, 37] is consistent with the available core-level spectroscopies. While the present calculations provide a good description of the experimental core-level spectra of NdNiO$_2$, we cannot explain the qualitative difference between the reported NdNiO$_2$ and LaNiO$_2$ XAS and RIXS spectra.

ACKNOWLEDGMENTS

We thank M. Kitatani, K. Yamagami, T. Uozumi, H. Ikeno, L. Si, M.-J. Huang and R.-P. Wang for valued discussions. A.H., M.W., and J.K. were supported by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (Grant Agreement No. 646807-EXMAG). A.H. was supported by JSPS KAKENHI Grant No. 21K13884.
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