Late transition-metal oxides with infinite-layer structure: nickelate vs. cuprate

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The correlated electronic structure of the infinite-layer compounds NdNiO$_2$ and SrCuO$_2$ at stoichiometry and with finite hole doping is compared. Key differences are elucidated from tackling the problem by a combination of density functional theory (DFT), self-interaction correction (SIC) and dynamical mean-field theory (DMFT) in the DFT+sicDMFT approach. While SrCuO$_2$ is verified as a charge-transfer insulator at strong coupling, a robust insulating regime remains absent in self-doped NdNiO$_2$ even for large interaction strength, though the transition-metal $d_{z^2-\gamma^2}$ spectral weight becomes generally gapped in that limit. A notable hybridization between Ni(3d) and Nd(5d) is crucial for the appearance of the self-doping band. Supercell calculations provide access to realistic hole-doping effects. Whereas Sr$_{1-y}$CuO$_2$ shows the expected hole-doped cuprate signatures, the absence of significant Zhang-Rice physics as well as a doping-dependent $d_{z^2}$-versus-$d_{x^2-y^2}$ competition at low-energy is revealed for Nd$_{1-x}$Sr$_x$NiO$_2$.

Introduction.— The competing energy scales of charge-transfer and on-site Coulomb kind are important for various properties of transition-metal (TM) oxides$^{11}$ including high-temperature superconductivity in doped layered cuprates.$^{2}$ Recently, Li et al. reported superconductivity up to $T_c = 15 \text{K}$ in the infinite-layer (IL) nickelate NiNdO$_2$ with hole doping.$^3$ It was achieved by thin-film generation via soft-chemistry topotactic reduction on a SrTiO$_3$ substrate. Albeit these results are debated in view of the underlying structural details,$^{12}$ this first successful finding of a respectable superconducting regime in conjunction with a layered-cuprate analogon from the nickelate family is remarkable.$^{13,14}$

The IL architecture usually refers to perovskite(-like) ABO$_n$ crystals in which the apical oxygens are missing, hence BO$_2$ square lattices are stacked with separating A layers. Transition-metal oxides of IL kind are e.g. known for iron$^{13}$ nickel$^{16,17}$ and copper$^{18,20}$ compounds. Generally for late transition-metal oxides, the TM(3d) subshell of $t_{2g} = \{d_{xz}, d_{yz}, d_{xy}\}$ character is completely filled and orbitals from the $e_g = \{d_{z^2}, d_{x^2-y^2}\}$ sector are partially filled. Whereas most cuprates are prototypical charge-transfer insulators with a comparatively small charge gap, many nickelates also carry substantial Mott-Hubbard character. Furthermore, while IL cuprates host the common formal Cu$^{2+}$ oxidation state, as the perovskite compounds, IL nickelates formally host the uncommon Ni$^+$ oxidation state$^{22}$ when Ni$^{2+}$ is usually realized in other nickel oxides. Thus one expects crucial normal-state differences between IL cuprates and nickelates at stoichiometry and with finite doping, largely effecting also the superconducting instability.

In this paper, we focus on a qualitative comparison of the long-known cuprate SrCuO$_2$ with the isostructural nickelate NdNiO$_2$. The former compound is a charge-transfer insulator$^{22}$ and becomes a high-temperature superconductor upon doping and further alloying.$^{19,20}$ On the other hand, the measured conductivity$^3$ in the stoichiometric IL nickelate does not suggest a sizable charge gap. Our realistic many-body studies take care of the subtle interplay between charge-transfer and Mott-Hubbard physics in these late TM oxides by including electronic correlations on TM and oxygen sites. It reveals important differences between both compounds, and points for NdNiO$_2$ toward a coexistence of Mott-critical layers with residual metallicity due to a subtle coupling between NiO$_2$ and Nd sheets. Upon hole doping, the stronger Mott-Hubbard character of the nickelate at low energy becomes evident, different from the Zhang-Rice physics of the cuprate.

Theoretical approach.— We employ the charge self-consistent combination$^{23}$ of density functional theory (DFT), self-interaction correction (SIC) and dynamical mean-field theory (DMFT) in the so-called DFT+sicDMFT framework$^{24}$. There, the TM sites of Ni or Cu chemical entity enter as DMFT impurities, while correlations on O are treated within SIC on the pseudopotential level.$^{25}$ The DFT part consists of a mixed-basis pseudopotential code$^{25,26}$ and the SIC is applied to

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**FIG. 1.** (color online) DFT band structure of NdNiO$_2$ (left) and SrCuO$_2$ (right) along high-symmetry lines in the Brillouin zone. Color coded are the dominant orbital weights (right) along high-symmetry lines in the Brillouin zone. Color coded are the dominant orbital weights (right) along high-symmetry lines in the Brillouin zone.
the 2s and the 2p orbitals of oxygen via weight factors \( w_p \) (see Ref. [25] for more details). Whereas the O(2s) orbital is by default fully corrected with \( w_p = 1.0 \), the common choice [21], [22] \( w_p = 0.8 \) is applied to the O(2p) orbitals. Note furthermore, that we put the Nd(4f) states in the pseudopotential core. Continuous-time quantum Monte Carlo in hybridization expansion [23] as implemented in the TRIQS code [20], [21] is utilized to solve the DMFT problem. In the DMFT correlated subspace, a five-orbital full Slater-Hamiltonian is applied to the TM-projected-local orbital [32]. All many-body calculations are performed in the paramagnetic regime for the system temperature \( T = 193 \text{ K} \). Maximum-entropy and Padé methods are employed for the analytical continuation from Matsubara space onto the real-frequency axis. Stoichiometric lattice parameters are overestimated from experiment [31], [32].

**Stoichiometric case.** — Figure 1 displays the nonmagnetic DFT band structures based on the local density approximation (LDA) for NdNiO\(_2\) and SrCuO\(_2\). Generally, the TM(3d) levels are closest to the Fermi level \( \varepsilon_F \), while the dominant part of O(2p) lies deeper in energy. The oxygen 2p levels are much more intertwined with TM(3d) in the cuprate compound, pointing to a stronger charge-transfer character of SrCuO\(_2\). We estimate the charge-transfer energy from \( \Delta = \varepsilon_d - \varepsilon_p \), where \( \varepsilon_d \) amounts to the average TM(3d) level and \( \varepsilon_p \) to the average O(2p) level, both computed from DFT+SIC [21]. This results in \( \Delta_{\text{NdNiO}_2} = 5.0 \text{ eV} \) and an indeed much lower \( \Delta_{\text{SrCuO}_2} = 1.3 \text{ eV} \). Similar calculations for rocksalt NiO resulted in \( \Delta_{\text{NiO}} = 4.5 \text{ eV} \) [22]. While the cuprate displays a single-sheet Fermi surface of dominant Cu-\( d_{x^2-y^2} \) character, a second band crosses \( \varepsilon_F \) in NdNiO\(_2\), giving rise to electron pockets at the Γ point and the A point. In both compounds, the Fermi sheets overlap and enclose a volume corresponding to one electron. The additional weakly-filled band in the nickelate has mixed character of mainly Nd-\( d_{x^2-y^2} \) and Ni-\( d_{z^2} \) around Γ as well as of Nd-\( d_{xy} \) and Ni-\( d_{xz} \), Ni-\( d_{yz} \) around A. It marks the self-doped nature of the IL nickelate. Similar hybridizations around Γ and A may also be observed in the cuprate case, along with the parallel contributions of Sr-\( d_{xz} \) and Sr-\( d_{xy} \). However there, the corresponding band above the dominant Cu-\( d_{x^2-y^2} \) dispersion does not cross the Fermi level. In terms of Ni-\( e_g \) based nearest-neighbor hoppings \( t \) to Nd-\( d_{xy} \) as extracted in a wide-energy picture, values read \( t_{\text{Nd}-d_{xy}} = 18 \text{ meV} \) and \( t_{\text{Nd}-d_{z^2}} = -69 \text{ meV} \). Such hoppings between Ni-\( d_{x^2-y^2} \) and Nd-\( d_{3z^2-r^2} \) are zero. The additional low-energy relevance of Ni-\( d_{z^2} \) from the \( e_g \) sector in IL nickelates has already been emphasized by Lee and Pickett [21]. Note also that the TM(4s) level hybridizes over a rather larger energy range, with appreciable weight at the O(2p)-block bottom, close to \( \varepsilon_F \) and again well above the Fermi level. It does not play a rele-

**FIG. 2.** (color online) DFT+sicDMFT spectral data of NdNiO\(_2\) (top,a-c) and SrCuO\(_2\) (bottom,d-f). (a,d) Total spectral function for \( U = 5, 10, 15 \text{ eV} \) (insets: low-energy blow up) joint with the TM(3d) occupation \( n_d \). (b,e) orbital- and site-projected spectral functions (upper part), and local TM-\( e_g \) spectral functions (lower part) joint with respective fillings \( n \). (c,f) \( k \)-resolved spectral function \( A(k, \omega) \) along high-symmetry lines. (b,c) are based on \( U = 10 \text{ eV} \) and (e,f) on \( U = 15 \text{ eV} \).
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![Diagram](image)

**FIG. 3.** (color online) Interacting ($U = 10 \text{ eV}$) Fermi surface of NdNiO$_2$ in the $k_z = 0$ (left) and the $k_z = 0.5$ (right) plane of the Brillouin zone (green square).

vant role for the encountered nickelate fermiology.

For the realistic many-body description beyond LDA, we take up a pragmatic position concerning the local Coulomb parameters. In late TM oxides, a value $J_H = 1 \text{ eV}$ is a common choice for the Hund’s exchange. For the better-screened Hubbard $U$, a value of $10 \text{ eV}$ recently provided very good agreement between theory and experiment for stoichiometric as well as Li-doped NiO within DFT+sicDMFT. While some authors expect a smaller $U$ in IL nickelate, the value for cuprates is usually expected larger than for nickelates. Hence, we start with the three different values $U = 5, 10, 15 \text{ eV}$ to cover the principally possible interaction space.

Figures 2a,d show the total $k$-integrated spectral function from DFT+sicDMFT using the three different $U$ values for NdNiO$_2$ and SrCuO$_2$. The $O(2p)$ block is shifted to deeper energies by $\sim 1 \text{ eV}$ for the former compound, due to the underestimation of the charge-transfer energy $\Delta$ within LDA. As expected, the cuprate compound becomes insulating at large $U$ with a gap of about $1.5 \text{ eV}$, i.e. on the order of $\Delta$. For the present largest choice of $U$, there is still some minor in-gap weight close to zero energy. A large value of $U > 10 \text{ eV}$ is not unreasonable in extended DMFT schemes for cuprate yet antiferromagnetic ordering surely additionally supports gap opening. The nickelate compound avoids an insulating state even for $U = 15 \text{ eV}$, i.e. the self-doped character remains robust up to large interaction strengths. Notably, the TM-$d_{x^2-y^2}$ weight is essentially gapped for NdNiO$_2$ at $U = 10 \text{ eV}$ and for SrCuO$_2$ at $U = 15 \text{ eV}$, which from that viewpoint renders the nickelate more strongly correlated. The TM(3$d$) occupation $n_g$ approaches the formal $d^9$ value in both cases with growing $U$. To proceed with further details, we narrow down the range of $U$ values to a single one for each compound via comparison to experiment: SrCuO$_2$ is a verified charge-transfer insulator, thus $U = 15 \text{ eV}$ is chosen; NdNiO$_2$ appears only weakly conducting, therefore we discard $U = 5 \text{ eV}$, and stick to $U = 10 \text{ eV}$ as a well-established value for nickelates. For the rest of the paper, these two choices should ensure a qualitatively reliable comparison of the correlated electronic structure of both compounds.

The orbital- and site projected spectral functions in Figs. 2e,f underline the different $O(2p)$ position in the nickelate and the cuprate. In the case of SrCuO$_2$, the lower Hubbard band (around $12 \text{ eV}$) lies well below $O(2p)$, whereas for NdNiO$_2$ (around $9 \text{ eV}$) it is located in the deeper-energy part of $O(2p)$. Both materials display sizable charge-transfer character, but with much stronger fingerprint in SrCuO$_2$. The charge-transfer signature in NdNiO$_2$ is weaker as e.g. in NiO. Both TM-$t_{2g}$ contributions, i.e. $x^2-y^2$ and $z^2$, are gapped for SrCuO$_2$, while the $z^2$ character takes part in the self-doped state, along with Nd(5$d$), in the case of the nickelate. At $U = 10 \text{ eV}$, the $x^2-y^2$ orbital in NdNiO$_2$ still marks contributions at lower energy, which are finally completely gone for $U = 15 \text{ eV}$. The $e_g$ occupations show that Ni-$d_{z^2}$ is indeed further away from complete filling than Cu-$d_{z^2}$, and hence more susceptible to charge fluctuations. Thus, a novel variant of orbital selectivity emerges, with localized Ni-$d_{z^2}$ and weakly-itinerant Ni-$d_{x^2}$ thanks to hybridization with Nd-$d$ in a self-doped manner. Though coupling between localized and itinerant electrons via inter-orbital effects on Ni is evident, a straightforward Kondo picture for localized Ni-$d_{z^2}$-$p^2$ does seemingly not apply. The $k$-resolved spectral functions in Figs. 2e,f confirm the previous statements on cuprate gap, nickelate self doping, and TM(3$d$) vs. $O(2p)$ position. Furthermore, in the NdNiO$_2$ case the $dd$-coupling of Ni-$e_g$ to Nd is favored for the self-doped band: compared to the LDA result which locates the electron pocket at $A$ deeper in energy, the many-body calculation intensifies the stronger Ni-$d_{z^2}$-to-Nd-$d_{z^2}$ hybridized electron pocket at $\Gamma$. Finally, the plotted nickelate Fermi surface in Fig. 3 displays circle-shaped sheets around $\Gamma$ and $A$.

**Hole-doped case.**— Let us turn to the electronic states with hole doping. The doped cases are realized by $2 \times 2 \times 2$ supercells of the nickelate and cuprate unit cells, respectively. This amounts to eight TM sites in the primitive cell, compared to only one in the stoichiometric unit cell. In the nickelate, Nd atoms are replaced by Sr atoms by a fraction $x$, while in the cuprate, Sr vacancies are generated by a fraction $y$. For Nd$_{1-x}$Sr$_x$NiO$_2$, two supercells are constructed: replacing on Nd atom ($x = 0.125$), and replacing two Nd atoms ($x = 0.250$). For Sr$_x$CuO$_2$, one vacant Sr site is introduced ($y = 0.125$). The atomic positions in the defect supercells are structurally relaxed within DFT+$U$. Notably, since each Sr vacancy gives rise to two holes, the actual doping level $\delta$ amounts to $\delta = x = 2y$. Note also again that we are here interested in principle effects and differences, and a very thorough many-body study of late quasi-twodimensional TM oxides at finite doping will ask for correlation effects beyond single-site DMFT (see e.g. Refs. 34 and 35 for reviews).

Figure 4 displays the spectral properties of the three hole-doping scenarios. In all cases, the electronic spectrum is shifted upwards in energy with doping, in line with available experimental data for IL cuprates. The doped charge-transfer insulator shows in Fig. 4e the spectral signature expected from a hole-doped cuprate.
filling of the gap and a resonance at $\varepsilon_F$, both with a substantial contribution from O(2$p$) states. Comparing the occupation numbers, $\delta_{\text{Cu}} = n_{\text{udoped}} - n_{\text{doped}} = 0.10$ holes per site are located on copper, while $\delta_{\text{O}} = \delta - \delta_{\text{Cu}} = 0.15$ holes per site are attributed to oxygen. The low-energy resonance marks the itinerant Zhang-Rice singlet physics.\(^{[37]}\). Hence, on the local Cu(3$d$) level, only the $x^2 - y^2$ orbital is contributing to the low-energy resonance. The situation is more intriguing for Nd(5$d$) (cf. Fig. 4a,b). First, significant low-energy Zhang-Rice physics cannot readily be identified, the spectrum close to $\varepsilon_F$ is strongly Ni(3$d$) dominated. Comparing the occupation numbers as before, a much larger relative hole count of $\delta_{\text{Ni}} = 0.09$ for $x = 0.125$ and of $\delta_{\text{Nd}} = 0.22$ for $x = 0.250$ on the TM site is obtained. Second, while for $x = 0.125$ the $x^2 - y^2$ orbital is mainly susceptible to doping, for $x = 0.250$ the $z^2$ orbital takes over in dominancy in this respect. This would result in a $x^2 - y^2$ vs. $z^2$ multi-orbital competition at the experimental $x = 0.2$ scenario for superconductivity.\(^{[13]}\)

The prominent $z^2$ role can be understood from the favorable hybridizations already established at stoichiometry. Note that the self-doped band itself is depleted already for small doping and traces of this may still be observed for $x = 0.125$ about 150 meV above $\varepsilon_F$. Further small-$\delta$ studies are necessary to map out this process in more detail.

**Summary and discussion.**— There are key differences between the infinite-layer TM oxides NdNiO$\text{2}$ and SrCuO$\text{2}$. The cuprate is a charge-transfer insulator at strong coupling, whereas the nickelate remains a non-insulating, self-doped system even at large interaction strength. Still, in both system the TM-$d_{x^2-y^2}$ state is half-filled localized (or very close to such a regime). In the IL architecture it is naturally expected that the missing apical oxygens allow for novel/modified hybridization scenarios for the TM(3$d$) orbitals with the surrounding. In the cuprate case, this does not lead to major qualitative changes compared to the perovskite case, since hybridization with non-oxygen orbitals leads states too high in energy to effect low-energy properties. On the other hand for rare-earth nickelates, the 5$d$ orbitals of the rare-earth ion enable low-energy hybridization with Ni(3$d$), i.e., additional band-crossing at $\varepsilon_F$ from self-doping. The Fermi surface becomes multi-sheeted, but still encompassing one electron. At strong coupling, where experiment seemingly places the material in the $d_{x^2-y^2}$ dominated sheet becomes gapped, but Luttinger theorem ensures the survival of the self-doped sheet.

For hole doping, the role of the self-doped band becomes minor for sizable dopings. However, a strong TM(3$d$)-O(2$p$) coupling at low energy is absent for the nickelate, and furthermore, $x^2 - y^2$ and $z^2$ compete close to the Fermi level. On the other hand, hole-doped SrCuO$\text{2}$ displays the expected $x^2 - y^2$ dominance even for the present overdoped scenario in view of superconductivity. One may speculate if the reduced $T_c$ for the nickelate compared to cuprates may be the result of that competition. For instance, due to loss of coherence in the interplay between two rather differently characterized orbital settings. On the other hand, the effective single-TM(3$d$) orbital together with the strong Zhang-Rice physics would then be key to the high $T_c$ of cuprates.

Further studies on IL nickelates and akin systems are highly desirable to fathom the designing options in view of raising $T_c$. In this context, the route along the metal-insulator transition in the oxygen-deficient LaNiO$_{3-x}$ perovskite for $x \geq 0.25$ with apparent oxygen-vacancy ordering is also noteworthy.\(^{[25,40]}\)

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