Effect of epitaxial strain on the electronic structure and magnetic correlations in infinite-layer (Nd,Sr)NiO$_2$

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We present a theoretical study of the effect of electron-electron interactions and Sr doping on the electronic structure of infinite-layer (Nd,Sr)NiO$_2$ using the density functional+dynamical mean-field theory approach. In particular, we explore the impact of epitaxial compressive strain that experience (Nd,Sr)NiO$_2$ films on the electronic properties, magnetic correlations, and exchange couplings. Our results reveal the crucial importance of orbital-dependent correlation effects in the Ni 3$d$ shell of Sr-doped NdNiO$_2$. Upon doping with Sr, it undergoes a Lifshitz transition which is accompanied by a reconstruction of magnetic correlations: For Sr $x < 0.2$ (Nd,Sr)NiO$_2$ adopts the Néel (111) antiferromagnetic (AFM) order, while for $x > 0.2$ the $C$-type (110) AFM sets in the unstrained (Nd,Sr)NiO$_2$, with a highly frustrated region at $x \approx 0.2$, all within DFT+DMFT at $T = 290$ K. Our results for the Néel AFM at Sr $x = 0$ suggest that AFM NdNiO$_2$ appears at the verge of a Mott-Hubbard transition, providing a plausible explanation for the experimentally observed weakly insulating behavior of NdNiO$_2$ for Sr $x < 0.1$. We observe that the Lifshitz transition makes a change of the band structure character from electron- to hole-like with Sr $x$, in agreement with recent experiments. Our results for magnetic couplings demonstrate an unanticipated frustration of the Ni 3$d$ magnetic moments, which suppresses magnetic order near Sr $x = 0.2$. We find that the effect of frustration is maximal for Sr doping $x \approx 0.1 - 0.2$ that nearly corresponds to the experimentally observed doping value. We conclude that the in-plane strain adjusts a bandwidth of the Ni $x^2 - y^2$ band, i.e., controls the effect of electron correlations in the Ni $x^2 - y^2$ orbitals. It suppresses the static $C$-type (110) ordering in (Nd,Sr)NiO$_2$ for Sr $x > 0.2$. Moreover, the in-plane strain affects the character of the Fermi surface of Sr-doped NdNiO$_2$ near the Brillouin zone A point, adjusting the crossover from electron- to hole-like behavior at high Sr $x$. The electronic structure and magnetic correlations of (Nd,Sr)NiO$_2$ reveal an anomalous sensitivity upon a change of the crystal structure parameters.

I. INTRODUCTION

The microscopic mechanism of unconventional high-$T_c$ superconductivity in cuprates, iron-based pnictides and chalcogenides remains a subject of intense research [1-5]. The recent discovery of superconductivity in nickel oxide-based materials, in the Sr-doped infinite-layer nickelate NdNiO$_2$, with a critical temperature up to $T_c \sim 15$ K suggests the possibility of a new family of nickelate superconductors analogous to copper oxides and iron-based superconductors [6,8]. This discovery has stimulated intensive efforts in understanding of the electronic structure of (Nd,Sr)NiO$_2$. While the infinite-layer parent compound NdNiO$_2$ share the same nominal transition metal 3$d^8$ configuration and crystal structure to those of cuprate CaCuO$_2$ (the latter exhibits superconductivity below $T_c \sim 110$ K upon hole doping [9,11]), the electronic states of NdNiO$_2$ reveal significant distinctions. Similar to the cuprates the low-energy physics of Sr-doped NdNiO$_2$ is dominated by electrons in the planar Ni $x^2 - y^2$ orbitals; these orbitals however experience strong hybridization with the Nd 5$d$ orbitals (primarily the $3z^2 - r^2$ and $xy$ orbitals), yielding a non-cuprate-like Fermi surface [12,15]. Yet, the possible importance of the Nd 4$f$ states has been pointed out, while these studies lead to conflicting conclusions, suggesting a Kondo-like (antiferro) [16] and anti-Kondo (ferro) Nd 4$f$-5$d$ exchange coupling [13]. In similarity to cuprates (Nd,Sr)NiO$_2$ shows a superconducting dome, although over a narrower doping window for Sr $0.125 < x < 0.25$ [7]. But in contrast to a Mott insulator for the underdoping and to a metal for the overdoping cuprates, in (Nd,Sr)NiO$_2$ it is bounded by a weakly insulating behavior on both sides of the dome. Moreover, unlike the antiferromagnetic insulator observed in undoped cuprates, yet there is no evidence for a magnetically ordered ground state in the undoped/or overdoped (Nd,Sr)NiO$_2$ [6,7]. Based on the experiments two features that are central to copper oxides – the Zhang-Rice singlet states and large planar spin fluctuations – were claimed to be absent (or diminished) in (Nd,Sr)NiO$_2$ [6,8]. This raises the important questions about the mechanism of superconductivity in the infinite-layer (Nd,Sr)NiO$_2$, which remain a subject of intense debates.

Although the electronic structure and magnetic properties of NdNiO$_2$ has recently been widely discussed based on applications of band structure methods [14] [17-25], model techniques [16, 29, 27], and density functional+dynamical mean-field theory (DFT+DMFT) [28,51] methods [30,34], the properties of Sr-doped NdNiO$_2$ are still poorly understood. For NdNiO$_2$, DFT+DMFT calculations reveal significant correlation effects within the Ni 3$d$ orbitals, which are complicated by large hybridization with the Nd 5$d$ states [15, 33-30]. DFT+DMFT calculations reveal a remarkable orbital-
selective renormalization of the Ni 3d bands, suggesting orbital-dependent localization of the Ni 3d states. Moreover, it was shown that (Nd, Sr)NiO$_2$ undergoes a Lifshitz transition of the Fermi surface which is accompanied by a change of magnetic correlations [13]. Most importantly, magnetic couplings in (Nd, Sr)NiO$_2$ were found to demonstrate strong frustration, which suppresses a static magnetic order, implying the importance of in-plane spin fluctuations to explain its superconductivity.

Experimentally, the superconducting (Nd, Sr)NiO$_2$ films were achieved by thin-film generation via soft-chemistry topotactic reduction of the perovskite NdNiO$_3$ to the infinite-layer phase deposited on a SrTiO$_3$ substrate [9–44]. This results in a compression of the unit-cell of NdNiO$_2$ in the $ab$ plane and its concurrent expansion along the $c$-axis. The latter is also due to partial substitution of Nd with a larger Sr ion [45]. In the previous DFT and DFT+DMFT works the primary focus was paid to a comparative study of the electronic structure of NdNiO$_2$ and CaCuO$_2$. While in a number of applications the effect of Sr doping of NdNiO$_2$ has been discussed, however, only the epitaxially (un-) strained crystalline state of (Nd, Sr)NiO$_2$ was considered. Thus, the role of the epitaxial strain and its effect on the electronic properties of (Nd, Sr)NiO$_2$ still needs to be understood on a microscopic level.

Here, we examine this subject using the state-of-the-art DFT+DMFT method implemented with plane-wave pseudopotentials [45–47]. DFT+DMFT has been proven to be among the most advanced theoretical methods for studying the electronic properties of strongly correlated materials, such as correlated transition metal oxides, heavy-fermions, and Fe-based superconductors, e.g., to study the phenomena of a Mott transition, collapse of local moments, large orbital-dependent renormalizations, etc. [45–60]. We use this advanced computational method to explore the effects of electronic correlations and Sr doping on the electronic structure, magnetic correlations, and exchange couplings of the unstrained (Nd, Sr)NiO$_2$. We compare our results with those previously obtained by us for (Nd, Sr)NiO$_2$ with the strained crystal structure [45]. We observe that the electronic structure and magnetic correlations of (Nd, Sr)NiO$_2$ reveal an anomalously sensitivity with respect to a change of the crystal structure parameters. We obtain that NdNiO$_2$ makes a Lifshitz transition, accompanied by a reconstruction of magnetic correlation, upon Sr doping $x \simeq 0.2$. Our results for magnetic couplings demonstrate an unanticipated frustration of the Ni 3d magnetic moments, which suppresses magnetic order near Sr $x = 0.2$, implying the importance of in-plane spin fluctuations to explain its superconductivity. We conclude that the in-plane strain adjusts a bandwidth of the Ni $x^2-y^2$ band, i.e., controls the effect of electron correlations in the Ni $x^2-y^2$ orbitals in (Nd, Sr)NiO$_2$.

II. COMPUTATIONAL DETAILS

We employ the state-of-the-art fully self-consistent in charge density DFT+DMFT method [20, 35] to examine the effects of electron correlations and Sr doping on the electronic structure and magnetic properties of infinite-layer (Nd, Sr)NiO$_2$. In particular, we focus on the effect of the epitaxial compressive strain that experience (Nd, Sr)NiO$_2$ on the SrTiO$_3$ substrate and discuss its effect on the electronic properties, magnetic correlations, and exchange coupling of bulk (Nd, Sr)NiO$_2$. In our study, we employ the unstrained crystal structure of bulk NdNiO$_2$, with the lattice parameters $a = 3.962$ Å and $c = 3.268$ Å (space group $P4/mmm$) obtained from structural optimization of NdNiO$_2$ within the DFT+U method [44–61] (the used values are within a ±1% from those obtained in experiment [44]). We note that for the Nd$_{0.2}$Sr$_{0.8}$NiO$_2$ film grown on the SrTiO$_3$ substrate the experimental lattice parameters are $a = 3.91$ Å and $c = 3.37$ Å (space group $P4/mmm$) [6]. We focus on the intrinsic magnetic instability in (Nd, Sr)NiO$_2$ caused by the Ni 3d electrons. In fact, the Nd 4f states in (Nd, Sr)NiO$_2$ are known to locate far away from the Fermi level (the effective interaction $U$ for the Nd 4f is about 10 eV). Because of this the low-energy physics of (Nd, Sr)NiO$_2$ is mainly governed by the effects of electronic correlations in the Ni 3d orbitals, which hybridize with the Nd 5d states. We therefore use La$_{3+}$ instead of the Nd$^{3+}$ (4f$^3$) ion in order to avoid the numerical instabilities arising from the Nd 4f electrons [19, 27, 57]. Hereafter, we assume La by saying Nd in our calculations.

To explore the effect of Sr doping on the electronic structure of (Nd, Sr)NiO$_2$ we use a fractional occupation within DFT that is often referred to as a rigid band approximation. We note that we employ a rigid-band shift of the Fermi level within DFT (not in the DFT+DMFT) and then compute the DFT+DMFT equations [28, 29]. That is, we perform a full solution of the DMFT equations for non-integer occupations leading to the self-consistent redistribution of the electronic spectral weight that allows us to capture the genuine many-body effects caused by interactions and doping. In our calculations we neglect the ionic radii mismatch between Nd and Sr ions.

In DFT we use the generalised gradient approximation for the correlation exchange functional [62]. In our calculations the Brillouin zone integration is performed with a $12 \times 12 \times 12$ k-point mesh. In our DFT+DMFT calculations we explicitly include the Ni 3d, Nd 5d, and O 2p valence states, by constructing a basis set of atomic-centered Wannier functions within the energy window spanned by these bands [59, 63]. This allows us to take into account a charge transfer between the partially occupied Ni 3d, Nd 5d, and O 2p states, accompanied by the strong on-site Coulomb correlations of the Ni 3d electrons. We use the continuous-time hybridization expansion (segment) quantum Monte Carlo algorithm in order to solve the realistic many-body problem [66].
take the average Hubbard $U = 6$ eV and Hund’s exchange $J = 0.95$ eV as previously employed for rare-earth nickelates RNiO$_3$. Here, we use the fully localized double-counting correction, evaluated from the self-consistently determined local occupations. The Coulomb interaction is treated in the density-density approximation. The spin-orbit coupling is neglected in our calculations. The angle resolved spectra were evaluated from analytic continuation of the self-energy results using Padé approximants.

In order to analyse a degree of localization of the Ni 3d electrons of paramagnetic (PM) Sr-doped NdNiO$_2$ we compute the local spin-spin correlation function $\chi(\tau) = \langle \hat{m}_z(\tau)\hat{m}_z(0) \rangle$ within DMFT, where $\hat{m}_z(\tau)$ is the instantaneous magnetization on the Ni 3d site at the imaginary time $\tau$ [28-29]. Our results for the evolution of magnetic correlations and possible magnetic instabilities of (Nd,Sr)NiO$_2$ upon Sr doping are analyzed by calculating the momentum-resolved static susceptibility in the particle-hole bubble approximation, with the interacting lattice Green’s function evaluated within DFT+DMFT (see, e.g., Refs. [15, 55, 56, 70, 71]). Using the DFT and DFT+DMFT methods we compute the electronic structure of the ferromagnetic (FM), Néel (111), C-type (110), single-stripe (100), (001), and staggered dimer (11 $\frac{1}{2}$) AFM states of (Nd,Sr)NiO$_2$. We consider only collinear spin configurations. We note that in our spin-polarized DFT+DMFT calculations the non-magnetic DFT was employed. For the magnetically ordered states of (Nd,Sr)NiO$_2$ we compute magnetic exchange couplings within the spin-polarized DFT and DFT+DMFT using the magnetic force theorem [22-23].

### III. RESULTS AND DISCUSSION

#### A. Electronic structure of paramagnetic (Nd,Sr)NiO$_2$

We start by computing the electronic structure and magnetic properties of paramagnetic (Nd,Sr)NiO$_2$. In Fig. 1 we display the k-resolved spectra of PM (Nd,Sr)NiO$_2$ obtained by DFT+DMFT for different Sr $x$. Our results for the Néel (111) and C-type (110) AFM states are summarized in Sec. B. Overall, our results for the PM phase agree well with those previously published [15]. We observe that the in-plane compressive lattice strain does not qualitatively change the electronic structure and hence the quasiparticle Fermi surface of (Nd,Sr)NiO$_2$ for small Sr $x$. For comparison we refer to our results for the band structure obtained by DFT+DMFT for the strained crystal structure of (Nd,Sr)NiO$_2$ [15].

For Sr $x = 0$ the Ni 3d spectral weight is distributed from −3 to 2 eV, with the localized Ni $t_{2g}$ complex near −2 eV. The Ni $x^2 - y^2$ and $z^2 - r^2$ states form a quasi two-dimensional-like band with a flat Γ-X and Γ-Z branches just below the Fermi level, with a substantial broadening of the electronic states near $E_F$ due to the effects of electron-electron correlations. The latter is most evident for the Ni $x^2 - y^2$ states near the M and A Brillouin zone (BZ) points. In addition, we observe a band formed by the mixed Ni and Nd $3z^2 - r^2$ states crossing $E_F$ near the Γ point which gives rise to the elliptical electron Fermi surface (FS) centered at the BZ center (Γ point) [15]. The mixed Ni $xz/yz$ and Nd $xy$ orbitals form a parabolic-like band crossing the Fermi level near the A point, resulting in the FS centered at the A point. Our results for the band structure of (Nd,Sr)NiO$_2$ show quasi-two-dimensional holelike FS sheets with a predominant Ni $x^2 - y^2$ character, similar to cuprates, which are centered at the A-M BZ edge.

**FIG. 1:** k-resolved spectral function of PM (Nd,Sr)NiO$_2$ with the unstrained lattice geometry for Sr $x = 0$ (top), 0.2 (middle) and 0.4 (bottom) as obtained by DFT+DMFT at $T = 290$ K.

Upon Sr $x$ (hole) doping, at $x = 0.2$, the Ni and Nd $3z^2 - r^2$ electronic states near the Γ point are seen to shift above the Fermi level, resulting in a change of the FS topology, i.e., a Lifshitz transition [15]. It is accompanied by the disappearance of the electron-like FS at the Γ point, with the formation of the holelike structures near the R and A BZ points. We point out that the effect of Sr doping is nontrivial and is accompanied by a charge redistribution between the Ni 3d and Nd 5d orbitals. Hence, it cannot be considered as a simple rigid shift of the Fermi level of pure NdNiO$_2$ within DMFT. In particular, upon doping from Sr $x = 0$ to 0.4 our results show a slight decrease of the Ni 3d occupations from 0.59 to 0.54 (per spin-orbital) for the $x^2 - y^2$ and from 0.85 to 0.81 for the $3z^2 - r^2$ orbitals, respectively. It leads to a change of the total Wannier Ni 3d occupation by ~0.14, whereas the Nd 5d and O 2p occupancies drop by ~0.17 and 0.05, respectively.

Most importantly, our results suggest a change of the
band structure character from electron- to hole-like in (Nd,Sr)NiO$_2$ upon doping with Sr $x$. This behavior promotes a change of the Hall coefficient from negative to positive, in agreement with recent experiments [7]. We find that the electronic structure and FS of PM (Nd,Sr)NiO$_2$ with the unstrained lattice do closely resemble that of the in-plane compressed PM (Nd,Sr)NiO$_2$ [15, 37, 40]. It seems that the change from the in-plane strained to unstrained lattice results in the appearance of the holelike Ni 3$d$ states crossing the $E_F$ near the A point at Sr doping $x \simeq 0.2$. For the strained geometry it takes place only for $x \geq 0.4$. That is, the in-plane strain mainly affects the character of FS at the A point, shifting the crossover from electron- to hole-like behavior to higher Sr doping $x$.

In agreement with our previous DFT+DMFT results [15], we observe a strong orbital-dependent correlation effects in the Ni 3$d$ band of PM (Nd,Sr)NiO$_2$. In Fig. 2 we display our results for the quasiparticle mass enhancement of the partially occupied Ni $x^2 - y^2$ and $3z^2 - r^2$ states evaluated from the slope of the polynomial fit of the imaginary part of the self-energy $\Sigma(i\omega_n)$ at $\omega_n = 0$ $m^*/m = 1 - \partial \ln \Sigma(i\omega_n)/\partial \omega_n$. For $x = 0$ we obtain a large quasiparticle mass enhancement $m^*/m \sim 3.3$ for the Ni $x^2 - y^2$ orbitals, while for the Ni $3z^2 - r^2$ states it is significantly weaker, about $\sim 1.3$. Our results are close to those previously obtained for the in-plane strained PM (Nd,Sr)NiO$_2$, namely, $m^*/m \sim 3.0$ and 1.3 for the Ni $x^2 - y^2$ and $3z^2 - r^2$ states, respectively [15]. In fact, correlation effects in the Ni $x^2 - y^2$ band are by about 10% stronger in PM (Nd,Sr)NiO$_2$ with the unstrained lattice. The latter is consistent with the increase of the Ni $x^2 - y^2$ bandwidth caused by the in-plane strain. Moreover, this orbital-selective strong correlation behavior of the Ni $x^2 - y^2$ and $3z^2 - r^2$ states is in line with sufficiently different occupations of these orbitals. Indeed, for $x = 0$ the $x^2 - y^2$ orbitals are nearly half-filled (0.59 per spin-orbit), while the $3z^2 - r^2$ orbitals are almost fully occupied (0.85). Our results clearly highlight the crucial importance of electronic correlations in PM (Nd,Sr)NiO$_2$.

Upon doping with Sr, we observe a gradual decrease of mass renormalization of the Ni $x^2 - y^2$ bands to about $m^*/m \simeq 2.5$ for Sr $x = 0.4$ (see Fig. 2). In contrast to that correlation effects in the Ni $3z^2 - r^2$ band tend to slightly increase with Sr $x$, to $m^*/m \simeq 1.5$ for Sr $x = 0.4$. In addition, the Ni 3$d$ occupations slightly decrease from 0.59 to 0.54 (per spin-orbit) for the $x^2 - y^2$ and from 0.85 to 0.81 for the $3z^2 - r^2$ orbitals for Sr $x = 0.4$, respectively. We notice no qualitative changes in the self-energy in PM (Nd,Sr)NiO$_2$ upon varying the Sr content $x$. The Ni 3$d$ states obey a Fermi-liquid-like behavior with a weak damping at the Fermi energy. Moreover, doping with Sr does not affect much magnetic moments in the PM phase of (Nd,Sr)NiO$_2$. In particular, upon changing of Sr $x$ from $x = 0$ to 0.4 the instantaneous local moments $\sqrt{m_z^2}$ increase only little, by about 4%, from 1.12 $\mu_B$ to 1.17 $\mu_B$. On the other hand, the orbital resolved contributions in the local moments exhibit qualitatively different behavior for the Ni $x^2 - y^2$ and $3z^2 - r^2$ states (see Fig. 2). While the local moments originating from the Ni $x^2 - y^2$ orbitals decrease from 0.42 to 0.34 $\mu_B$, i.e., by $\sim 20\%$, the $3z^2 - r^2$ orbital moments rise by almost twice from 0.09 to 0.17 $\mu_B$. This behavior is consistent with the behavior of the orbital-dependent renormalizations $m^*/m$ of the Ni 3$d$ bands upon Sr doping. It explains a weak dependence of the local moments upon Sr doping $x$. In fact, the Ni $x^2 - y^2$ and $3z^2 - r^2$ local moments contributions almost cancel each other, resulting in a nearly constant $\sqrt{m_z^2}$ with Sr $x$. It is also seen from the nonmonotonous behavior of the fluctuating magnetic moments $M_{loc} = [T F_{m_z}^{1/2}(m_z(\tau))m_z(\tau)]^{1/2}$ (see Fig. 2). We note that in the strained (Nd,Sr)NiO$_2$ the fluctuating local moments are also weakly dependent on Sr $x$, $\sim 0.43$
and 0.41 $\mu_B$ for Se $x = 0$ and 0.4, respectively.

Next, we evaluate the local spin susceptibility $\chi(\tau) = \langle \hat m_x(\tau) \hat m_z(0) \rangle$ for the Ni 3$d$ orbitals and examine the orbital-dependent correlation effects in the Ni 3$d$ band of (Nd, Sr)NiO$_2$. Our results for $\chi(\tau)$ obtained by DFT+DMFT at $T = 290$ K ($\beta = 40$ eV$^{-1}$) for different Sr doping $x$ are shown in Fig. 3. Our analysis of the local spin susceptibility suggests the proximity of the heavily renormalized Ni $x^2 - y^2$ orbitals to localization, while the weakly renormalized $3z^2 - r^2$ states are delocalized. In particular, for the Ni $3z^2 - r^2$ states $\chi(\tau)$ is seen to decay fast to zero with the imaginary time $\tau$, which is typical for itinerant behavior. In contrast to that $\chi(\tau)$ for the $x^2 - y^2$ states is sufficiently larger, $\chi(0) = 0.73 \mu_B^2$, slowly decaying to $\sim 0.1 \mu_B^2$ at $\tau = \beta/2$. Overall, our results reveal that magnetic correlations in NdNiO$_2$ are at the verge of orbital-dependent formation of local magnetic moments. In agreement with this the calculated (instantaneous) magnetic moment of Ni is about 1.12 $\mu_B$, consistent with nearly a $S = 1/2$ state of nickel. Upon hole doping, correlation effects in the Ni $x^2 - y^2$ orbitals are weakened, in agreement with a significant decrease of the $x^2 - y^2$ derived local moments and decrease of the quasiparticle mass $m^*/m$. Our findings are consistent with the behavior of the strained (Nd, Sr)NiO$_2$. We propose that the in-plane strain affects a bandwidth of the in-plane Ni $x^2 - y^2$ band, adjusting the effect of electron correlations in the Ni $x^2 - y^2$ band in (Nd, Sr)NiO$_2$.

Our results suggest that the Lifshitz transition in (Nd, Sr)NiO$_2$ is accompanied by a change of the FS nesting and hence by a reconstruction of magnetic correlations. It appears near the experimentally observed doping for the superconducting dome in (Nd, Sr)NiO$_2$ Sr $x \simeq 0.2$. To check this, we proceed with an analysis of the symmetry and strength of magnetic correlations in (Nd, Sr)NiO$_2$. We determine the momentum-dependent static magnetic susceptibility $\chi(\tau)$ within DFT+DMFT using the particle-hole bubble approximation. In Fig. 4 we show orbitally resolved contributions to $\chi(\tau)$ along the highly-symmetric BZ path and their evolution upon doping with Sr. Our results for the total $\chi(\tau)$ are shown in Supplementary Fig. S1. We note that our results for $\chi(\tau)$ for the unstrained (Nd, Sr)NiO$_2$ agree qualitatively well with those for the in-plane strained (Nd, Sr)NiO$_2$. For Sr $x = 0$ within both DFT and DFT+DMFT $\chi(\tau)$ shows two leading magnetic instability for a wave vector $q_m = (111)$ and (110) that corresponds to the long-range Néel and C-type AFM ordering, respectively. It appears mainly from the Ni $x^2 - y^2$ orbital contribution. $\chi(\tau)$ for the $3z^2 - r^2$ states is small and nearly $q$-independent. In the same time, $\chi(\tau)$ for the Nd 5$d$ states reveals a weak ferromagnetic instability, which is seen as a weak anomaly at the $\Gamma$ point.

We find that $\chi(\tau)$ for the Néel AFM is higher than that for the C-type AFM. The latter is consistent with the total-energy calculations within the spin-polarized DFT and DFT+DMFT methods revealing that the Néel AFM ordering is more favorable for Sr $x = 0$ (see Fig. 5). On the other hand, $\chi(\tau)$ for Sr $x \geq 0.2$ $\chi(\tau)$ shows a change of magnetic correlations from the Néel (111) at $x < 0.2$ to the C-type (110) AFM at $x \geq 0.2$. In fact, for $x \geq 0.2$ $\chi(\tau)$ now predicts a leading magnetic instability at $q_m \simeq (110)$. It appears due to the Ni $3z^2 - r^2$ orbital contribution, while for the Ni $x^2 - z^2$ states $\chi(\tau)$ is nearly equal for the wave vectors (111) and (110). In the same time for Sr $x \geq 0.2$ Nd 5$d$ states show a nearly flat and $q$-independent $\chi(\tau)$. We note the importance of correlation effects. It is seen as a qualitative difference in $\chi(\tau)$ obtained by DFT and DFT+DMFT for $x \geq 0.2$. In particular, while for $x = 0.2$ DFT yields the Néel (111) state to be the most stable, the DFT+DMFT predicts the (110).

### B. Electronic structure of (Nd, Sr)NiO$_2$ in magnetically ordered state

![Energy difference diagram](image)

**FIG. 5:** Total energy difference $\Delta E = E_{\text{max}} - E_{\text{NM}}$ between the long-range magnetically ordered and non-magnetic states of NdNiO$_2$ as a function of hole doping Sr $x$ calculated by DFT (open symbols). Ferromagnetic (FM), Néel (111), C-type (110), single-stripe (100), staggered dimer (11½), and (001) AFM states are shown. DFT+DMFT results for the total energy difference between the Néel and C-type AFM states and the paramagnetic state at $T = 290$ K are depicted by solid symbols.
Next, we proceed with a detailed study of the electronic and magnetic structure of (Nd, Sr)NiO$_2$. Using the DFT and DFT+DMFT methods we compute the electronic structure for the spin-collinear ferromagnetic (FM), Néel (111), C-type (110), single stripe (100), (001), and staggered dimer (11$\frac{1}{2}$) AFM states of (Nd, Sr)NiO$_2$. Our results of the spin-polarized DFT and DFT+DMFT total energy and magnetization calculations are summarised in Figs. [5] and [6]. In fact, for Sr $x = 0$ the Néel AFM ordering is more energetically favorable by about 3 meV/f.u. with respect to the C-type AFM and the PM state within DFT+DMFT, at $T = 290$ K. The total energy difference is more pronounced (due to the absence of quantum spin fluctuations) within DFT, $\sim$106 meV/f.u. between the Néel (111), C-type (110), and (11$\frac{1}{2}$) and the non-magnetic ground state. Interestingly, for the strained (Nd, Sr)NiO$_2$ it is about 85 meV/f.u. [15].

For Sr $x = 0$ we found multiple magnetic solutions using both the DFT and DFT+DMFT methods. In contrast to DFT only the Néel, C-type (110), and staggered dimer (11$\frac{1}{2}$) AFM states are found to be stable within DFT+DMFT at $T = 290$ K, with a nearly equal magnetization of 0.74 $\mu$B/Ni (see our results for the magnetic moments obtained using the spin-polarized DFT+DMFT shown in Fig. [6]). In DFT these magnetic configurations are nearly degenerate in total energy, within $\sim$7 meV/Ni. Our results therefore point out that various types of spin order are competing (nearly degenerate in the total energy) in (Nd, Sr)NiO$_2$, implying frustration of the Ni 3$d$ magnetic moments. In agreement with this the momentum-dependent static magnetic susceptibility $\chi(q)$ exhibits a nearly-equal tendency towards the Néel and C-type AFM for small Sr $x$ (see Fig. [4]).

Upon doping with Sr, our results for $\chi(q)$ reveal a change of magnetic correlations from a three-dimensional Néel (111) to quasi-two-dimensional C-type (110). In agreement with our results for (Nd, Sr)NiO$_2$ with the in-plane strained lattice structure [15], near Sr $x \approx 0.2$ we observe a sharp suppression of the calculated magnetization $M_z$ and hence of the Néel temperature obtained within DFT+DMFT. For Sr $x = 0.2$ we find no evidence of a magnetically ordered state down to the lowest studied temperature $T = 116$ K. Thus, all magnetic configurations discussed here, namely, the FM and (100), (110), (111), and (11$\frac{1}{2}$) AFM collapse in the PM state. This suggests that for Sr $x \approx 0.2$ the Néel (Curie) temperature is sharply suppressed within DFT+DMFT. This implies a sufficient increase of quantum spin fluctuations near $x \approx 0.2$, i.e., Sr $x \approx 0.2$ can be interpreted as a quantum critical point [75, 76].

For Sr $x > 0.2$ we find that all the magnetic configurations discussed here, except the C-type (110), are unstable (i.e., collapse in the PM state) within DFT+DMFT at $T = 290$ K. We notice that the static C-type (110) AFM state is stable for Sr $x > 0.2$, with a magnetization of $\sim$0.32 $\mu$B/Ni at $x = 0.4$, in agreement with our DFT+DMFT results for the momentum-dependent static magnetic susceptibility $\chi(q)$ (see Fig. [4]). For the (110) AFM state within DFT+DMFT for Sr $x = 0.4$ we find a total energy gain of $\sim$27 meV/f.u. with respect to the PM state, at $T = 290$ K. Interestingly that our results for the strained (Nd, Sr)NiO$_2$ show no stable long-range C-type (110) AFM state for $x > 0.2$ at $T = 290$ K, implying that the in-plane strain suppress the static C-type (110) ordering in (Nd, Sr)NiO$_2$ [15]. Most importantly, we find that magnetization sharply collapses to the PM state for Sr $x \approx 0.2$ within DFT+DMFT, with a change of the magnetic state from the $q_m = (111)$ for $x < 0.2$ to (110) for $x > 0.2$. This result is consistent with the Lifshitz transition scenario at $x \approx 0.2$.

![FIG. 6: Long-range ordered magnetic moments of Ni as a function of Sr $x$ calculated for (Nd, Sr)NiO$_2$ by DFT (empty symbols). DFT+DMFT results for the Néel (111), C-type (110), and staggered dimer (11$\frac{1}{2}$) AFM states at $T = 290$ K are shown by filled symbols.](image)

![FIG. 7: k-resolved spectral function of (Nd, Sr)NiO$_2$ for the Néel Sr $x = 0$ (top) and C-type (110) $x = 0.4$ AFM (bottom) as obtained by DFT+DMFT at $T = 290$ K.](image)
The total spectral functions are shown in Supplementary Figs. S2 and S3. In our results reveal a drastic change of the electronic structure of (Nd,Sr)NiO$_2$ caused by magnetic ordering. In particular, for the Néel AFM at $x = 0$ we find that the Ni $x^2−y^2$ state is highly spin-polarized. Its majority spin occupancy is $\sim 0.93$, while for the Ni $x^2−y^2$ minority spin state it is only 0.25. For $x = 0$ the Ni 3$d$ magnetization is $0.74 \mu_B$. The nearly occupied Ni 3$z^2−r^2$ states are weakly spin-polarized with majority and minority spin occupations $\sim 0.89$ and 0.84, respectively.

The Ni $t_{2g}$ states are fully occupied and are localized at about $−2$ eV (see Fig. 8). The majority spin Ni $x^2−y^2$ states are located just below $E_F$ to $−3$ eV, with a peak at $\sim −0.16$ eV due to the (coherent) quasiparticle Ni $x^2−y^2$ states and the lower Hubbard subband (incoherent part) at about $−1$ eV. The “unoccupied” minority spin Ni $x^2−y^2$ states appear at $\sim 1$ eV above the Fermi level and show a substantial broadening caused by correlation effects. These states are seen as highly incoherent dispersive states with a bandwidth of about 2 eV just above $E_F$. In addition, the spin minority Ni $d_{x^2−y^2}$ states show a flat subband just above the Fermi level near the X-M-$\Gamma$ and R-A-M BZ paths due to the strong correlation self-energy effects. While in our analysis we employed the Páde analytical continuation procedure for the self-energy results, we find this behavior to be robust for different Páde approximants setups. We find that the broad parabolic-like partially filled bands crossing the Fermi level near the $\Gamma$ point are predominantly originated from the Nd 5$d$ orbitals, partly mixed with occupied the Ni $t_{2g}$ and 3$z^2−r^2$ states. Our results for the Néel AFM therefore suggest that the Ni 3$d$ bands are nearly gapped at the Fermi level due to correlation effects and magnetic ordering, implying that AFM NdNiO$_2$ is at the verge of a Mott-Hubbard transition. As a result, the total spectral function exhibits a pseudogap, providing a plausible interpretation for the experimentally observed weakly insulating behavior of NdNiO$_2$ for small Sr doping $x < 0.1$. This is in accordance with the previous DFT+DMFT results, suggesting that AFM NdNiO$_2$ undergoes a Mott-Hubbard transition, which takes place for the Ni Hubbard $U \geq 7$ eV [35][31]. We notice that a relatively small Nd 5$d$ Hubbard $U$ value may also affect the band structure of AFM NdNiO$_2$, resulting in a Mott-Hubbard insulating solution.

For Sr $x > 0.2$ (Nd,Sr)NiO$_2$ makes a phase transition in the $C$-type (110) AFM state. The phase transition results in a remarkable reconstruction of the electronic structure of (Nd,Sr)NiO$_2$ (see Figs. 1 and 7). For $x = 0.4$ the Ni 3$d$ magnetization is about $0.32 \mu_B$/Ni. Due to the hole doping, the Ni $x^2−y^2$ state is weakly spin-polarized with majority and minority spin occupancies of $0.64$ and 0.45, respectively. The Ni 3$z^2−r^2$ occupations are about 0.89 and 0.76 for the spin majority and minority states, respectively. In contrast to our results for $x = 0$, the Ni $x^2−y^2$ states for both spin projections cross the Fermi level. The “unoccupied” minority spin Ni 3$z^2−r^2$ states cross the Fermi energy near the M point and are located between $−0.5$ eV to 2 eV. They show a substantial broadening caused by correlation effects and are seen as highly incoherent dispersive states near to above $E_F$. The Ni 3$z^2−r^2$ majority spin states are nearly fully occupied, while the minority ones appear at $E_F$. The Ni $t_{2g}$ states are fully occupied and are localized near to about $−2$ eV below $E_F$ (see Fig. 8). While for the $x = 0$ Néel state the band structure of (Nd,Sr)NiO$_2$ is dominated by electron character, for Sr $x = 0.4$ it seems to be holelike. We propose that the Lifshitz transition makes a change of the band structure character from electron- to hole-like in (Nd,Sr)NiO$_2$ with Sr $x$.

To proceed further we compute magnetic exchange couplings within the spin-polarized DFT and DFT+DMFT using the magnetic force theorem [72][73][74]. Our results for the Néel and $C$-type (110) AFM states are summarized in Fig. 8. We observe that for Sr $x = 0$ the interlayer exchange coupling is small and weakly antiferromagnetic, $J_1 \sim −9$ K ($−25$ K in DFT), and ferromagnetic, 2 K (27 K), for the Néel and $C$-type (110) AFM states, respectively. The in-plane couplings $J_1$ (nearest-neighbor) and $J_2$ (next-nearest-neighbor) are
both antiferromagnetic and are sufficiently higher by modulus, -174/-30 K (-203/-35 in DFT) and -179/-33 K (-206/-39 K) for the Néel and C-type (110) AFM states, respectively. This result is in agreement with experimental estimates [78, 79].

In agreement with our previous results for the in-plane strained (Nd,Sr)NiO$_2$ [15], we observe a remarkable change of the $J_2/J_1$ ratio with respect to Sr $x$. It is increasing from 0.17 to 0.67 upon going from Sr $x = 0$ to 0.1 as obtained by DFT+DMFT for the Néel state. In DFT the change is more sluggish from 0.17 to 0.43 from Sr $x = 0$ to 0.3. In fact, we can interpret this behavior as a highly frustrated $J_2/J_1 \simeq 0.4$ - 0.5 region of a spin-$\frac{1}{2}$ frustrated $J_1$-$J_2$ Heisenberg model on the 2D square lattice realized in (Nd,Sr)NiO$_2$ upon doping with Sr [80-82]. In agreement with this, the DFT+DMFT magnetization is found to quickly collapse to the PM state for Sr $x \simeq 0.2$. In DFT this highly frustrated state seems to take place at $x = 0.3$. In addition, near $x = 0.05$ - 0.1 we observe a crossover in the 2D magnetic state with $J_\perp \simeq 0$ K [15, 37]. In close analogy with the spin-$\frac{1}{2}$ frustrated $J_1$-$J_2$ Heisenberg model where the highly frustrated region is sandwiched between the Néel and stripe type (or valence-bond solid) ordered states [80-82], in our case the frustration region is sandwiched between the two different long-range ordered antiferromagnets. This suggests that magnetic couplings in (Nd,Sr)NiO$_2$ near to an optimal doping demonstrate an unanticipated frustration, which suppresses a long-range magnetic order (resulting in a drastic drop of the Néel temperature).

Furthermore, our results for the exchange couplings obtained by DFT+DMFT for the C-type (110) AFM state for Sr $x = 0.5$ reveal a relatively large, dominating over the in-plane couplings, interlayer exchange coupling $J_\perp = -50$ K ($-136$ K in DFT). The $J_1$ and $J_2$ in-plane couplings are only $-11$ and $-6$ K ($-33$ and $-17$ K in DFT), respectively. This suggests that in the unstrained (Nd,Sr)NiO$_2$ the Lifshitz transition is accompanied by a change of magnetic couplings from the in-plane highly-frustrated quasi-2D to an effective quasi-1D AFM chain along the $z$-axis with weak in-plane interactions. Interestingly while $J_\perp$ is found to be dominating for Sr $x > 0.3$, it is insufficient to stabilize the (001) AFM state within DFT+DMFT. In particular, our spin-polarized DFT+DMFT calculations for the (001) AFM state for Sr $x = 0.5$ result in the PM state at $T = 290$ K, i.e., the (001) AFM was found to be unstable. Overall, our results point out high frustration of magnetic couplings in (Nd,Sr)NiO$_2$, implying that superconductivity in infinite-layer (Nd,Sr)NiO$_2$ appears to be similar to that observed in iron chalcogenides and pnictides [83-88]. Moreover, we note an anomalous sensitivity of the electronic structure and magnetic correlations of (Nd,Sr)NiO$_2$ with respect to the lattice structure. Our results suggest the importance of in-plane spin fluctuations to explain superconductivity in (Nd,Sr)NiO$_2$, in contrast to previous claims.

IV. CONCLUSION

In conclusion, we employed the DFT+DMFT computational approach to study the effects of electronic correlations and Sr doping on the electronic structure and magnetic properties of infinite-layer (Nd,Sr)NiO$_2$. In particular, we study the effect of the in-plane epitaxial strain that experience (Nd,Sr)NiO$_2$ films on the electronic properties, Fermi surface topology, magnetic correlations, and exchange coupling of bulk (Nd,Sr)NiO$_2$. Our results reveal the crucial importance of electronic correlations in (Nd,Sr)NiO$_2$. We observe a strong orbital-dependent correlation effects in the Ni 3d band of PM (Nd,Sr)NiO$_2$, implying that magnetic correlations in (Nd,Sr)NiO$_2$ are at the verge of orbital-dependent localization. Upon doping with Sr (Nd,Sr)NiO$_2$ is found to undergo a Lifshitz transition which is accompanied by a change of magnetic correlations. We found that magnetization sharply collapses to the PM state for Sr $x \simeq 0.2$ within DFT+DMFT, with the change of a magnetic state from the Néel (111) for $x < 0.2$ to (110) for $x > 0.2$. Sr $x \sim 0.2$ can be interpreted as a quantum critical point.
We observe that the Lifshitz transition makes a change of the band structure character from electron- to hole-like in (Nd,Sr)NiO$_2$ with Sr $x$, in agreement with recent experimental studies [7].

Our results for magnetic couplings demonstrate an unanticipated frustration of the Ni 3$d$ magnetic moments, which suppresses magnetic order near Sr $x \approx 0.2$. We find that the effect of frustration is maximal for Sr doping $x \approx 0.1 - 0.2$ that nearly corresponds to the experimentally observed doping value of (Nd,Sr)NiO$_2$. We conclude that the in-plane strain acts as a bandwidth control mechanism which adjusts correlation effects in the Ni $x^2 - y^2$ band in (Nd,Sr)NiO$_2$. It suppress the static C-type (110) ordering in (Nd,Sr)NiO$_2$ for Sr $x > 0.2$. The latter is found to be stable for the unstrained lattice of (Nd,Sr)NiO$_2$ at Sr $x = 0$ which suppresses magnetic order near Sr $x \approx 0.1 - 0.2$. Our results for the Néel AFM at Sr $x = 0$ suggest that AFM NdNiO$_2$ appears at the verge of a Mott-Hubbard transition, providing a plausible interpretation for the experimentally observed weakly insulating behavior of NdNiO$_2$ for Sr $x < 0.1$. We notice an anomalous sensitivity of the electronic structure and magnetic correlations of (Nd,Sr)NiO$_2$ with respect to the lattice structure. Our results suggest that superconductivity in nickelates is strongly influenced, or even induced, by in-plane spin fluctuations, while superconductivity in infinite-layer (Nd,Sr)NiO$_2$ appears to be similar to that observed in iron chalcogenides and pnictides.

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We note that the experimental estimates for bulk gives 26 meV.

The DFT total energy difference for the AFM and FM states give an uniform antiferromagnetic exchange coupling $\sum_{i>j} S_i S_j / |S| = 1/2$ notation of the Heisenberg model

Upon Sr doping.

We adopt the following notation for the Heisenberg model, $H = - \sum_{i<j} J_{ij} e_i e_j$, where $e_i$ are the unit vectors.

We note that the experimental estimates for bulk NdNiO$_2$ give an uniform antiferromagnetic exchange coupling $J \sim 25$ meV for NdNiO$_2$ written in the $H = J \sum_i S_i \cdot S_j$, $|S| = 1/2$ notation of the Heisenberg model [73]. Within the same notation, our estimate from the DFT total energy difference for the AFM and FM states gives 26 meV.

We also note the raw data for the experimental estimates for bulk NdNiO$_2$ gives an uniform antiferromagnetic exchange coupling $J \sim 25$ meV for NdNiO$_2$ written in the $H = J \sum_i S_i \cdot S_j$, $|S| = 1/2$ notation of the Heisenberg model [73]. Within the same notation, our estimate from the DFT total energy difference for the AFM and FM states gives 26 meV.
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Supplementary Material: Effect of epitaxial strain on the electronic structure and magnetic correlations in infinite-layer (Nd,Sr)NiO$_2$

FIG. S1: Static spin susceptibility $\chi(q)$ of Sr-doped NdNiO$_2$ as a function of hole doping Sr $x$ calculated by DFT+DMFT at $T = 290$ K.

FIG. S2: Total and orbitally resolved spectral functions of the Neél AFM ordered NdNiO$_2$ (Sr $x = 0$) as obtained by DFT+DMFT at $T = 290$ K.
FIG. S3: Total and orbitally resolved spectral functions of the C-type (110) AFM ordered (Nd,Sr)NiO$_2$ with Sr $x = 0.4$ as obtained by DFT+DMFT at $T = 290$ K.