Fingerprints of nematicity and competing orders in the infinite-layer nickelate

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Recent discovery of superconductivity in the nickelates has ignited renewed theoretical and experimental interest in the role of electronic correlations in their properties. Here, based on in-depth first-principles and many-body perturbation theory modeling, we show that the parent (undoped) compound of the nickelate family, LaNiO2, hosts competing low energy phases, unlike the undoped cuprates but similar to the case of the doped cuprates. We also show the existence of flat bands near the Fermi level, stemming from the Ni-3d orbitals, that are found to persist across the various predicted low-energy phases of the nickelates. Our study gives insight into the microscopic origin of electronic inhomogeneity and nematicity and lack of long-range order in the nickelates.

I. INTRODUCTION

Emergence of symmetry-breaking, competing low-energy phases driven by the complex interplay of spin, charge, orbital, and lattice degrees of freedom is a universal characteristic of correlated systems [1–3]. Examples are the unconventional superconductors, such as the cuprates [4–6], iron-based superconductors [7], and twisted bilayer graphene [8] are prominent examples, where a wide variety of experiments have revealed the presence of competing inhomogeneous orders and a rich tapestry of phase diagrams. Although the mechanism of high-temperature superconductivity remains elusive after 30 years of intense study, it is now generally accepted that competing orders play an important role in this connection [1–3].

Recent discovery of superconductivity in the hole-doped infinite-layer nickelates [9–12] has attracted intense attention [13–15] as an analog of cuprate superconductivity. Much experimental and theoretical effort has been devoted to understanding the relationship between the nickelates and cuprates [16–29]. It has been suggested that the nickelates are closer to the Mott-Hubbard limit due to the large Ni-3d and O-2p orbital splitting, in contrast to the charge-transfer case of the cuprates [16, 24, 25, 28, 29]. Although a variety of tight-binding models have been proposed [24, 30, 31] to understand the low-energy physics of the nickelates, the roles of various orbitals involved remain unclear.

The parent compound LaNiO2 of the nickelate family has been shown experimentally to exhibit strong antiferromagnetic (AFM) fluctuations and spin-glass behavior [32–34], competing charge orders [35, 36], and possible superconductivity [33, 37]. This is strikingly different from the case of the undoped cuprates, which assume a well-defined AFM ground state, but similar to the case of the doped cuprates. These similarities and differences between the cuprates and the nickelates have naturally raised many questions [13–15, 29]. For example, can the nickelates be described by a one-band model like the cuprates? Why is there no long-range magnetic order in the nickelates even at low temperature [34, 38–41]? Do nickelates host competing orders similar to those found in other unconventional superconductors, such as the stripe and nematic phases? Answers to these questions will likely also provide new clues for understanding the mechanism of high-Tc superconductivity.

Here, we discuss our first-principles calculations based on the density functional theory (DFT) and many-body perturbation theory for the parent compound LaNiO2 of the nickelate family. Besides being a prototypical infinite-layer nickelate, LaNiO2 has the added advantage of lacking complications arising from f-electrons. Our total energy calculations demonstrate the existence of a number of stripe-like phases with low energy in pristine LaNiO2, similar to the doped cuprates. Their total energies, magnetic moments, and electronic structures are delineated. The stripe phases are lower in energy than most of the non-stripe phases we reported earlier [29]; in fact, some stripes have lower energy than the previously reported C-type AFM (C-AFM) ground state, strikingly similar to the case of the doped cuprates [42]. Furthermore, in both the C-AFM and the stripe phases in the nickelates, the calculated band structures contain flat bands dominated by Ni 3d_{xz} orbitals near the Fermi level, inducing Van Hove singularities in the density of states (DOS), which could enhance many-body interactions and drive more exotic correlated phenom-
FIG. 1. Schematics of 1D bond- and site-centered stripes along the $a$-axis in LaNiO$_2$. (a) The bond-centered stripe phase with periodicity $P_c = P_m = 5$, where $P_m$ and $P_c$ denote the periodicities of the spin and charge orders, respectively. Here the antiphase boundaries (APBs) pass through the bonding oxygen atoms. (b) The site-centered stripe phase with $P_m = 8$ and $P_c = 4$. The APB passes through the Ni atoms. The blue and yellow circles represent Ni and O atoms, respectively. La atoms are omitted in the figure for clarity. The green arrows indicate the relative orientation of magnetic moments on Ni atoms, and the red lines with double arrows point to the APBs.

Our many-body theory calculations confirm these findings and suggest the existence of incommensurate stripe phases that are not accessible to DFT-based modeling. Our findings here provide insight into the low-energy physics and the lack of long-range magnetic order in the nickelates.

II. METHODS

First principles calculations were performed by using the pseudopotential projector-augmented wave method [44] as implemented in the Vienna ab initio simulation package (VASP) [45, 46]. A high-energy cutoff of 520 eV was used to truncate the plane-wave basis set. The exchange-correlation effects were treated using the strongly-constrained-and-appropriately-normed (SCAN) [47] density functional. Crystal structures and ionic positions were fully optimized in all cases using a force convergence criterion of 0.01 eV/Å for each atom along with a total energy tolerance of $10^{-5}$ eV. The unfolded band structures including orbital characters were extracted from the supercell pseudowavefunction calculations [48] using PyProcar [49] and Pymatgen [50] software. The random phase approximation (RPA) calculation of the spin and orbital fluctuations was performed by employing a real-space tight-binding model Hamiltonian, which was obtained by using the VASP2WANNIER90 [51] interface. For LaNiO$_2$, the full manifolds of Ni-3$d$, La-5$d$, and La-4$f$ states were included in generating the Wannier functions. The response functions were evaluated over a $51 \times 51 \times 51$ $k$-mesh at 0.001 $K$, using the 4 bands at the Fermi level in the sum over bands in the Lindhard susceptibility, along with a finite broadening of 0.005 eV [52, 53].

Our RPA-type calculations are restricted to considering only local interactions similar to the multiorbital Hubbard model [54] as presented in Ref. 52. The charge and spin response ($\delta \rho$, $\delta \pi$) of the system to an infinitesimal perturbing source field is given by a generalized RPA-type matrix equation,

\[
\chi^{MN}(q, \omega) = \left[1 - \chi_0^{MI}(q, \omega)\nu^{IK}\right]^{-1}\chi_0^{KN}(q, \omega),
\]

\[
= \left[1 - \tilde{F}^{MK}(q, \omega)\right]^{-1}\chi_0^{KN}(q, \omega),
\]

where, for brevity, the orbital indices have been suppressed. To make the various charge and spin instabilities of the system apparent, we diagonalize the kernel $\tilde{F}$,

\[
\tilde{F} = V^\dagger(q, \omega)\lambda_F(q, \omega)V(q, \omega)
\]
where $\Lambda_F$ is a diagonal matrix, and $V$ is unitary. Then
\begin{equation}
\chi^{MN}(q, \omega) = V_{M\alpha}^\dagger(q, \omega) \left[ 1 - \Lambda_F^\alpha(q, \omega) \right]^{-1} V_{\alpha K} \chi_{KN}^0(q, \omega),
\end{equation}
where $\alpha$ enumerates the instability eigenmodes. As $\Lambda_F^\alpha(q, \omega = 0)$ approaches 1 the ground state becomes unstable to an ordered phase. Additionally, the momentum satisfying $\Lambda_F^{\alpha_{\text{max}}}(q, \omega = 0) = 1$, where $\alpha_{\text{max}}$ is the index of the maximum eigenmode, is the propagating vector $Q$ of the emerging Stoner instability in the multiorbital spin-dependent system. The character of this instability may then be obtained by analyzing the associated eigenvectors, $V$. See Ref. 52 for details. Here we used a critical on-site Coulomb potential strength of $1.22$ eV to access the leading Stoner instability of the system.

### III. RESULTS

#### A. Possible Stripe Phases in LaNiO$_2$

After low-energy stripe phases were first reported in cuprates [4–6], considerable effort has been devoted to studying the connection between inhomogeneous states and superconductivity. In this respect, it is important to study competing orders in the nickelates and determine similarities and differences with cuprates. Here, to search more low-energy states, we consider two typical stripe phases in our calculations. One is a bond-centered 1-dimensional (1D) stripe phase, where the antiphase boundaries (APBs) pass through the Ni-O-Ni bond, i.e., centered on the O. The other one is 1D site-centered stripe order, where the APBs pass through Ni atoms. Schematic plots of these stripes are shown in Fig. 1. Fig. 1(a) depicts a stripe of charge periodicity of $P_c = 5$ on Ni atoms, and magnetic order of periodicity $P_m = 5$. After relaxation, our calculations find that there are no obvious lattice distortions around the APBs, with only very small shifts of the oxygen atomic positions toward the APBs, exhibiting amplitudes of $\sim 0.005$ Å. The calculated magnetic moments of Ni atoms are around $1.06 \mu_B$ with small modulations of $\sim 0.022 \mu_B$, leading to a slightly enhanced magnetic density around the APBs. Figure 1(b) presents a 1D site-centered stripe order with charge and magnetic periodicity of $P_c = 4$ and $P_m = 8$, respectively. Notably, we find the self-consistent magnetic moment of each Ni atom along the APBs to be $0 \mu_B$, whereas the Ni atoms away from the APB exhibit a $1.00 \mu_B$ moment in site-centered cases. $P_c$’s of site-centered stripe phase we considered are 3, 4, 5, 6, 7, and 9. However, for bond-centered ones, $P_c$ we studied are 3, 4, 5, 6, 7, 9 and 11. Computations for larger values of $P_c$ become impractical.

Notably, there is a significant charge redistribution between the two configurations in real space around the AFM-stripe phase boundary. To make this point clear, we plot the charge density difference between C-AFM and selected stripe phases in Figures S1 (Supplementary Material). Interestingly, a stronger charge redistribution is observed in site-centered stripe phase, due to the larger energy difference between C-AFM and site-centered phases, which we will defer in next section. A part of the charge redistribution in the bond-centered stripe phase is contributed by La orbitals as shown in Fig. S1 (a), which indicates that additional orbitals may play a role in the low-energy physics in nickelates.
B. Stripe Ground States

The absence of long-range magnetic order in nickelates suggests the existence of strong spin fluctuations. To better understand this point, we calculate the total energies of a number of 1D stripe phases as a function of charge periodicity. Figure 2 reveals striking similarities with cuprates, despite some differences. Figure 2 (a) shows the total energies of each site and bond centered stripe state for undoped LaNiO$_2$ relative to the C-AFM phase [29]. Our total energy calculations show the bond-centered phases to be the more stable compared to the site-centered stripes, consistent with results on cuprates [42]. Moreover, we find that the bond-centered stripes become more stable as the charge periodicity increases, consistent with pristine YBa$_2$Cu$_3$O$_6$ (YBCO) [42].

Figure 2 (b) compares the total energy of the various magnetic phases with the average Ni magnetization. Here, we include all of the 1D stripe phases up to $P_c = 11$, along with a variety of uniform magnetic phases previously reported [29] using the C-AFM phase as the reference. Overall, we find a larger average Ni magnetic moment results in a more stable magnetic phase. In particular, multiple phases with strong local magnetic moments are found to be nearly degenerate in energy, with quite small energy differences less than 3 meV. This result is in remarkable agreement with our recent study of the yttrium-based cuprates [42], which revealed that “intertwined orders” with larger magnetic moment are crucial for understanding the propieties of correlated materials. Notably, we rule out any significant role of the non-magnetic (NM) phase in the ground state since it is not energetically competitive ($\sim$400 meV). We emphasize that, similar to the doped cuprates, Fig. 2 clearly provides evidence of the existence of competing low-energy states in LaNiO$_2$.

We find one significant difference, namely that in undoped cuprates the stripe phases are always metastable, with excess energy $\sim 1/P_c$, leading to a well-defined AFM ground state [42], whereas in the nickelates the stripes appear close to becoming the lowest energy states—similar to YBCO$_7$ [42]. This suggests that the nickelates may be closer to the Slater regime, where fermi surface nesting can lower the stripe energy. This enhanced stripe-AFM competition may explain why LaNiO$_2$, like YBCO$_7$, has no long-range magnetic order [9, 40].

C. RPA Calculations

In YBCO$_7$, there is a minimum energy charge periodicity [42], whereas in nickelates the energy appears to be decreasing monotonically with $P_c$. To explore the full manifold of possible stripe phases and search for a minimum stripe energy, we perform an RPA instability analysis on the NM state.

D. Electronic Structures

The preceding analysis suggests that the competing low-energy orders are essential for understanding the properties of LaNiO$_2$. Therefore, to understand the
infinite-layer nickelates we need to consider the ensemble of magnetic and stripe states, but not the NM phase. To gain insight into the electronic properties of the ground state, we examine the electronic band structures of a bond-centered stripe and the uniform C-AFM phase.

**FIG. 4. Comparison of the electronic structures of C-AFM and bond-centered stripe phases.** (a) Orbitally-projected electronic structures of C-AFM phase. (b) Same as (a), but for the bond-centered phase with \( P_c = P_m = 5 \) stripe. Both band structures are “unfolded” onto the primitive \( 1 \times 1 \times 1 \) Brillouin zone. The site-projected orbitally-resolved partial densities of states are for Ni sites with positive magnetic moment.

Figure 4 presents the unfolded electronic band structures of LaNiO\(_2\) in the C-AFM (a) and \( P_c = P_m = 5 \) bond-centered stripe (b) phases, respectively. As pointed out in Ref. [29], the magnetic state appears as a Hund’s phase, where the magnetic moments primarily consist of \( d_{x^2-y^2} \) character (0.75\( \mu_B \)), with a smaller admixture from \( d_{z^2} \) (0.25\( \mu_B \)). This is reflected in the band structure. The Ni-\( d_{x^2-y^2} \) band (red) is fully gapped out, and the \( d_{z^2} \) is spin-split (blue), similar to the cuprates [56]. Due to the fractional filling of the upper Ni-\( d_{z^2} \) band, it is pinned to the Fermi level producing a flat band in the \( k_z = \pi \) plane, consistent with previous studies [29, 43]. Similar results are found for the \( P_c = P_m = 5 \) stripe (0.78 \( \mu_B \) from \( d_{x^2-y^2} \), 0.26 \( \mu_B \) from \( d_{z^2} \)). Remarkably, this pinning is absent in the NM phase, and arises from a strong reorganization of the \( d_{z^2} \) dispersion when a magnetic gap opens on the \( d_{x^2-y^2} \) band. This two-dimensional flat band gives rise to a higher-order (1D) Van Hove singularity (VHS) in the DOS, which can enhance the many-body interaction and drive more exotic correlated phenomena [57]. This flat band has also been suggested to couple electronic and lattice instabilities [29, 43]. However, it is extremely rare to find a VHS exactly at the Fermi level, without driving a transition to a new phase.

Upon unfolding the unit cell to capture the \( P_c = P_m = 5 \) stripe, we find the resulting band dispersions [Figs. 4(b)] are only slightly modified from that of the C-AFM phase. Specifically, the degeneracy of bands in the stripe phase gets lowered due to the reduction in symmetry within the stripe phase. Despite the lower symmetry, the 3\( d_{z^2} \) flat band is preserved, pinned to the Fermi level in the stripe phase, which generally exists in the low-energy phases of LaNiO\(_2\) as we show in Sec. 2 of the SM. Away from the Fermi level, minigaps form in the Ni-3\( d_{z^2} \)/La-\( d \) hybridized band due to the supermodulation of the crystal potential, typical of stripe-like structures [58]. This is also consistent with cuprates, where the stripes were identified as topological defects of an underlying AFM order.

In contrast to the cuprates, LaNiO\(_2\) differs from the insulating cuprate parent compounds in that the former is a metal, with partially filled Ni 3\( d_{z^2} \), 3\( d_{x^2-y^2} \), and La 5\( d \) hybridized bands, indicating that a multiorbital model is necessary to properly describe the role of valence fluctuations between Ni\(^{2+} \) (\( \delta^6 \)) and Ni\(^{1+} \) (\( \delta^7 \)). The behavior of the magnetic state is similar to the cuprates, except for a somewhat larger energy scale. That is, the magnetic gaps in the Ni-\( d_{x^2-y^2} \) band is approximately double that in the cuprates owing to the larger magnetic moments. Consequently, the energetic ordering scale of magnetic and stripe states in Fig. 2(b) is a factor of 5-7 larger than those in YBCO\(_7\) [42].

**IV. DISCUSSION**

Despite significant differences between cuprates and nickelates, there is a great deal of similarity between the results of Fig. 2 and those of Figs. 2 and 3 for YBCO in Ref. 42. We suggest that this similarity is a signature of strong correlations being at play in correlated materials that are realized as a form of short-range order in which topological defects—here domain walls—play a significant role. Topological defects are also known to play an important role in Martensitic phases [59] and in quenches [60].

It has been postulated that high-\( T_c \) superconductivity could arise simply by tipping the balance between the competing orders, or it could actually benefit from the presence of the strongly correlated and the bad metal Slater phase [57, 61]. The present study based on DFT and many-body theory provides direct evidence for the existence of electron correlation effects and exotic states in undoped nickelates.

Our findings support the experimental observation of fluctuating magnetic effects in nickelates [21, 31, 33–36, 38–41]. We find nearly degenerate orders of bond-
centered stripes and C-AFM phases, along with flat bands in the low-energy region around the Fermi energy. Additional competing spin and charge orders are suggested by our many-body theory calculations, which could lead to intertwined orders in pristine LaNiO$_2$. Spin fluctuations associated with such nearly degenerate states could play a significant role in driving superconductivity, as suggested for other unconventional superconductors [1–3]. This could also explain superconductivity in undoped LaNiO$_2$ [33, 37]. A doping dependent study is needed to fully elucidate this connection.

It is interesting that no obvious lattice distortion is found in our bond-centered stripe calculations, suggesting that spin-phonon coupling may not be important for driving superconductivity in pristine LaNiO$_2$. This needs to be confirmed by further theoretical and experimental studies. Our DFT and many-body calculations, however, indicate a striking similarity between the undoped nickelates and doped cuprates.

Our results show that both charge and spin orders should be observable in experiments, although only charge orders have been reported so far in the literature [33, 35, 36]. In fact, fluctuating unidirectional stripes could lead to in-plane electronic anisotropy (i.e. nematicity). Therefore, a local probe, such as scanning tunneling microscopy, may help unravel the relationship between the charge and spin density orders predicted by our computations.

V. CONCLUSION

Using first principles calculations based on DFT and many-body perturbation theory, we provide clear evidence for the presence of correlated low-energy phases stabilized by magnetic moments as well as the existence of VHSs in the nickelates, much like the doped cuprates. Our findings highlight the striking similarities between the undoped nickelates and doped cuprates. The Ni 3d$_z^2$ orbital is found to lie close to the Fermi energy, indicating that it could play an important role in superconductivity and that a multi-orbital minimal model is needed to capture the physics of the nickelates accurately.

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